DOCUMENTATION OF THE SAPRC99 CHEMICAL MECHANISM FOR VOC REACTIVITY ASSESSMENT

DRAFT
Report to California Air Resources Board
Contract 92-329

By

William P. L. Carter

April 27, 1999

Air Pollution Research Center and
College of Engineering
Center for Environmental Research and Technology
University of California
Riverside, California 92521

98-AP-RT17-001-FR

TABLE OF CONTENTS

LIST OF TABLES

II. CHEMICAL MECHANISM COMPONENTS

The major components of the SAPRC mechanisms are the base mechanism, the mechanism and parameters for the detailed model species, and the lumping procedures. The base mechanism is the portion of the mechanism used to represent the reactions of the inorganic species, the common organic products, the intermediate radicals leading to these products, including those formed from the initial reactions of the detailed model species. The detailed model species are used to represent most of the emitted VOCs, which are not in the base mechanism. These can be added to the mechanism (either as explicit reactions for individual VOCs or as lumped model species whose parameters are derived from the mixture of detailed model species they represent), as needed in the model application. The detailed model species include those that have explicit rate constant and product yield parameters assigned for all their relevant atmospheric reactions, and those, which are represented by other model species using "lumped molecule" assignments.

In this section we discuss the components of the mechanism that are derived from chemical mechanistic considerations. This includes the base mechanism and those detailed model species for which kinetic and mechanistic parameters have been derived. The evaluation of these components of the mechanism against environmental chamber data is then discussed in the following section. After that, the lumping procedures used to represent complex mixtures, and other considerations involved when implementing this mechanism in airshed calculations are discussed.

A. Base Mechanism

The base mechanism is the portion of the mechanism which must be incorporated when representing the reactions of any generic VOC, and includes the inorganic reactions, the reactions of the common organic products and the reactions of the common radicals formed from these products or any generic VOC. A complete listing of the base mechanism is given on Tables 1-3, with the species used in the base mechanism listed on Table 1, their reactions and rate constants listed on Table 2, and the absorption cross sections and quantum yields for the photolysis reactions listed on Table 3. Footnotes to Table 2 give the documentation for the reactions and rate constants in the mechanism. The major features of the mechanisms, and the changes made relative to the previous version (Carter et al, 1997a) are discussed in the following sections.

1. Inorganic Reactions

The inorganic reactions in the mechanism are essentially the same as in the previous versions, except all the rate constants have been updated based on the results of the most recent evaluations (Atkinson et al, 1997a,b, 1999; Atkinson, 1997a; NASA, 1997). This resulted in changes to most of the rate constants, though in most cases the changes were small probably not of significance to model predictions. In addition, a few reactions that were previously judged to be negligible were added to extend the range of validity of the mechanism. The changes that may not be negligible, and the aspects of the inorganic mechanism that are still considered to be uncertain, are briefly summarized below, in the order that the reactions appear on Table 2.

Table 1. Listing of model species used in the base mechanism

Name	Description
Constant Species.	
O2	Oxygen
M	Air
H2O	Water
HV	Light
Active Inorganic Species.	
O3	Ozone
NO	Nitric Oxide
NO2	Nitrogen Dioxide
NO3	Nitrate Radical
N2O5	Nitrogen Pentoxide
HONO	Nitrous Acid
HNO3	Nitric Acid
HNO4	Peroxynitric Acid
HO2H	Hydrogen Peroxide
CO	Carbon Monoxide
SO2	Sulfur Dioxide
Active Radical Species and Operators.	
HO.	Hydroxyl Radicals
HO2.	Hydroperoxide Radicals
C-O2.	Methyl Peroxy Radicals
RO2-R.	Peroxy Radical Operator representing NO to NO2 conversion with HO2 formation.
R2O2.	Peroxy Radical Operator representing NO to NO2 conversion.
RO2-N.	Peroxy Radical Operator representing NO consumption with organic nitrate formation.
CCO-O2.	Acetyl Peroxy Radicals
RCO-O2.	Peroxy Propionyl and higher peroxy acyl Radicals
BZCO-O2.	Peroxyacyl radical formed from Aromatic Aldehydes
MA-RCO3.	Peroxyacyl radicals formed from methacrolein and other acroleins.
Steady State Radical Species	
O3P	Ground State Oxygen Atoms
O*1D2	Excited Oxygen Atoms
TBU-O.	t-Butoxy Radicals
BZ-O.	Phenoxy Radicals
BZ(NO2)-O.	Nitro-substituted Phenoxy Radical
HOCOO.	Radical formed when Formaldehyde reacts with HO2
PAN and PAN Analogues	
PAN	Peroxy Acetyl Nitrate
PAN2	PPN and other higher alkyl PAN analogues
PBZN	PAN analogues formed from Aromatic Aldehydes
MA-PAN	PAN analogue formed from Methacrolein
Explicit and Lumped Molecule Reactive Organic Product Species	
HCHO	Formaldehyde
CCHO	Acetaldehyde
RCHO	Lumped C3+ Aldehydes
ACET	Acetone

Table 1 (continued)

Name	Description
MEK	Ketones and other non-aldehyde oxygenated products which react with OH radicals slower than 5×10^{-12} cm^3 $molec^{-2}$ sec^{-1}.
MEOH	Methanol
COOH	Methyl Hydroperoxide
ROOH	Lumped higher organic hydroperoxides
GLY	Glyoxal
MGLY	Methyl Glyoxal
BACL	Biacetyl
PHEN	Phenol
CRES	Cresols
NPHE	Nitrophenols
BALD	Aromatic aldehydes (e.g., benzaldehyde)
METHACRO	Methacrolein
MVK	Methyl Vinyl Ketone
ISOPROD	Lumped isoprene product species
Lumped Parameter Products	
PROD2	Ketones and other non-aldehyde oxygenated products which react with OH radicals faster than 5×10^{-12} cm^3 $molec^{-2}$ sec^{-1}.
RNO3	Lumped Organic Nitrates
Uncharacterized Reactive Aromatic Ring Fragmentation Products	
DCB1	Reactive Aromatic Fragmentation Products that do not undergo signficant photodecomposition to radicals.
DCB2	Reactive Aromatic Fragmentation Products which photolyze with alpha-dicarbonyl-like action spectrum.
DCB3	Reactive Aromatic Fragmentation Products which photolyze with acrolein action spectrum.
Non-Reacting Species	
CO2	Carbon Dioxide
XC	Lost Carbon
XN	Lost Nitrogen
SULF	Sulfates (SO_3 or H_2SO_4)
H2	Hydrogen
Low Reactivity Compounds or Unknown Products Represented as Unreactive	
HCOOH	Formic Acid
CCO-OH	Acetic Acid
RCO-OH	Higher organic acids
CCO-OOH	Peroxy Acetic Acid
RCO-OOH	Higher organic peroxy acids
CONO2	Methyl Nitrate
NROG	Unspecified Unreactive Carbon
Primary Organics Represented explicitly	
CH4	Methane
ISOPRENE	Isoprene

Table 2. Listing and documentation of the reactions in the base mechanism.

Label	Rate Parameters [a]				Refs &	Reaction and Products [b]
	k(300)	A	Ea	B	Notes	
Inorganic Reactions						
1	Phot Set= NO2				1,2	NO2 + HV = NO + O3P
2	5.91e-34	5.91e-34	0.00	-2.8	3	O3P + O2 + M = O3 + M
3	8.34e-15	8.00e-12	4.09		4,5	O3P + O3 = #2 O2
4	1.00e-31	1.00e-31	0.00	-1.6	6,7,5	O3P + NO + M = NO2 + M
5	9.70e-12	6.50e-12	-0.24		4,5	O3P + NO2 = NO + O2
6	1.79e-12	Falloff, F=0.80			4,7,5	O3P + NO2 = NO3 + M
	0:	9.00e-32	0.00	-2.0		
	inf:	2.20e-11	0.00	0.0		
8	1.87e-14	1.80e-12	2.72		6	O3 + NO = NO2 + O2
9	3.72e-17	1.40e-13	4.91		6	O3 + NO2 = O2 + NO3
10	2.60e-11	1.80e-11	-0.22		6	NO + NO3 = #2 NO2
11	1.93e-38	3.30e-39	-1.05		6	NO + NO + O2 = #2 NO2
12	1.53e-12	Falloff, F=0.45			6,7	NO2 + NO3 = N2O5
	0:	2.80e-30	0.00	-3.5		
	inf:	2.00e-12	0.00	0.2		
13	6.74e-2	Falloff, F=0.45			6,7	N2O5 = NO2 + NO3
	0:	1.00e-3	21.86	-3.5		
	inf:	9.70e+14	22.02	0.1		
14	2.60e-22	2.60e-22			8	N2O5 + H2O = #2 HNO3
15		(Slow)			9	N2O5 + HV = NO3 + NO + O3P
16		(Slow)			9	N2O5 + HV = NO3 + NO2
17	6.75e-16	4.50e-14	2.50		10	NO2 + NO3 = NO + NO2 + O2
18	Phot Set= NO3NO				1,11,12	NO3 + HV = NO + O2
19	Phot Set= NO3NO2				1,11,12	NO3 + HV = NO2 + O3P
20	Phot Set= O3O3P				1,13,14	O3 + HV = O3P + O2
21	Phot Set= O3O1D				1,13,14	O3 + HV = O*1D2 + O2
22	2.20e-10	2.20e-10			4	O*1D2 + H2O = #2 HO.
23	2.87e-11	2.09e-11	-0.19		15	O*1D2 + M = O3P + M
24	7.31e-12	Falloff, F=0.60			16	HO. + NO = HONO
	0:	7.00e-31	0.00	-2.6		
	inf:	3.60e-11	0.00	-0.1		
25	Phot Set= HONO-NO				1,17,18	HONO + HV = HO. + NO
26	Phot Set= HONO-NO2				1,17,18	HONO + HV = HO2. + NO2
27	6.42e-12	2.70e-12	-0.52		6	HO. + HONO = H2O + NO2
28	8.81e-12	Falloff, F=0.60			19	HO. + NO2 = HNO3
	0:	2.43e-30	0.00	-3.1		
	inf:	1.67e-11	0.00	-2.1		
29	2.00e-11	2.00e-11			6,20	HO. + NO3 = HO2. + NO2
30	1.44e-13	5.45e-15	-1.95		21,22	HO. + HNO3 = H2O + NO3
31	Phot Set= HNO3				1,23	HNO3 + HV = HO. + NO2
32A	1.30e-13	1.30e-13			24	HO. + CO = HO2. + CO2
32B	3.19e-33	3.19e-33			24	HO. + CO + M = HO2. + CO2 + M
33	6.78e-14	1.90e-12	1.99		6	HO. + O3 = HO2. + O2
34	8.36e-12	3.40e-12	-0.54		6	HO2. + NO = HO. + NO2
35	1.36e-12	Falloff, F=0.60			6	HO2. + NO2 = HNO4
	0:	1.80e-31	0.00	-3.2		

Table 2. Listing and documentation of the reactions in the base mechanism.

Label	Rate Parameters [a]				Refs & Notes	Reaction and Products [b]
	k(300)	A	Ea	B		
	inf:	4.70e-12	0.00	0.0		
36	9.61e-2	Falloff, F=0.50			6	HNO4 = HO2. + NO2
	0:	4.10e-5	21.16	0.0		
	inf:	5.70e+15	22.20	0.0		
37	Phot Set= HO2NO2				1,25	HNO4 + HV = #.61 {HO2. + NO2} + #.39 {HO. + NO3}
38	4.98e-12	1.50e-12	-0.72		6	HNO4 + HO. = H2O + NO2 + O2
39	1.89e-15	1.40e-14	1.19		6	HO2. + O3 = HO. + #2 O2
40A	1.63e-12	2.20e-13	-1.19		26	HO2. + HO2. = HO2H + O2
40B	3.48e-30	3.08e-34	-5.56		26	HO2. + HO2. + H2O = HO2H + O2 + H2O
40C	4.85e-32	1.85e-33	-1.95		26	HO2. + HO2. + M = HO2H + O2 + M
40D	1.04e-49	2.59e-54	-6.32		26	HO2. + HO2. + M + H2O = HO2H + O2 + M + H2O
41	4.00e-12	4.00e-12			27	NO3 + HO2. = HO. + NO2 + O2
42	2.41e-16	8.50e-13	4.87		28	NO3 + NO3 = #2 NO2 + O2
43	Phot Set= H2O2				1,29	HO2H + HV = #2 HO.
44	1.70e-12	2.90e-12	0.32		6	HO2H + HO. = HO2. + H2O
45	1.10e-10	4.80e-11	-0.50		6	HO. + HO2. = H2O + O2
S2OH	4.00e-31	Falloff, F=0.45			6,30	HO. + SO2 = HO2. + SULF
	0:	2.00e-12	0.00	0.0		
	inf:	4.00e-31	0.00	-3.3		
Methyl peroxy and methoxy reactions						
MER1	7.24e-12	2.80e-12	-0.57		31,32	C-O2. + NO = NO2 + HCHO + HO2.
MER4	5.12e-12	3.80e-13	-1.55		31	C-O2. + HO2. = COOH + O2
MEN3	1.30e-12	1.30e-12			31	C-O2. + NO3 = HCHO + HO2. + NO2
MER5	2.61e-13	2.45e-14	-1.41		33	C-O2. + C-O2. = MEOH + HCHO + O2
MER6	1.08e-13	5.90e-13	1.01		33	C-O2. + C-O2. = #2 {HCHO + HO2.}
Peroxy Racical Operators						
RRNO	8.96e-12	2.70e-12	-0.72		34,35,32	RO2-R. + NO = NO2 + HO2.
RRH2	1.45e-11	1.90e-13	-2.58		35,36	RO2-R. + HO2. = ROOH + O2 + #-3 XC
RRN3	2.30e-12	2.30e-12			37,38	RO2-R. + NO3 = NO2 + O2 + HO2.
RRME	2.00e-13	2.00e-13			39,40	RO2-R. + C-O2. = HO2. + #.75 HCHO + #.25 MEOH
RRR2	3.00e-14	3.00e-14			41,40	RO2-R. + RO2-R. = HO2.
R2NO	Same k as rxn RRNO				42,43	R2O2. + NO = NO2
R2H2	Same k as rxn RRH2				42,43	R2O2. + HO2. = HO2.
R2N3	Same k as rxn RRN3				42,43	R2O2. + NO3 = NO2
R2ME	Same k as rxn RRME				42,43	R2O2. + C-O2. = C-O2.
R2RR	Same k as rxn RRR2				42,43,40	R2O2. + RO2-R. = RO2-R.
R2R3	Same k as rxn RRR2				42,43	R2O2. + R2O2. =
RNNO	Same k as rxn RRNO				42,44	RO2-N. + NO = RNO3
RNH2	Same k as rxn RRH2				42,44,45	RO2-N. + HO2. = ROOH + #3 XC
RNME	Same k as rxn RRME				42,44,46	RO2-N. + C-O2. = HO2. + #.25 MEOH + #.5 {MEK + PROD2} + #.75 HCHO + XC
RNN3	Same k as rxn RRN3				42,44,47	RO2-N. + NO3 = NO2 + O2 + HO2. + MEK + #2 XC
RNRR	Same k as rxn RRR2				42,44,46	RO2-N. + RO2-R. = HO2. + #.5 {MEK + PROD2} + O2 + XC

Table 2. Listing and documentation of the reactions in the base mechanism.

Label	Rate Parameters [a]				Refs &	Reaction and Products [b]
	k(300)	A	Ea	B	Notes	
RNR2	Same k as rxn RRR2				42,43	RO2-N. + R2O2. = RO2-N.
RNRN	Same k as rxn RRR2				42,44,46	RO2-N. + RO2-N. = MEK + HO2. + PROD2 + O2 + #2 XC
Reactions of Acyl Peroxy Radicals, PAN, and PAN analogues						
APN2	1.04e-11	Falloff, F=0.30			48	CCO-O2. + NO2 = PAN
		0:	2.70e-28	0.00	-7.1	
		inf:	1.20e-11	0.00	-0.9	
DPAN	7.04e-4	Falloff, F=0.30			49	PAN = CCO-O2. + NO2
		0:	4.90e-3	24.05	0.0	
		inf:	4.00e+16	27.03	0.0	
APNO	2.18e-11	2.18e-11			50	CCO-O2. + NO = C-O2. + CO2 + NO2
APH2	1.38e-11	4.30e-13	-2.07		51	CCO-O2. + HO2. = #.75 {CCO-OOH +O2} + #.25 {CCO-OH + O3}
APN3	4.00e-12	4.00e-12			52	CCO-O2. + NO3 = C-O2. + CO2 + NO2 + O2
APME	9.53e-12	1.80e-12	-0.99		53	CCO-O2. + C-O2. = CCO-OH + HCHO + O2
APRR	1.00e-11	1.00e-11			54,55	CCO-O2. + RO2-R. = CCO-OH
APR2	Same k as rxn APRR				42,43	CCO-O2. + R2O2. = CCO-O2.
APRN	Same k as rxn APRR				42,55,46	CCO-O2. + RO2-N. = CCO-OH + PROD2
APAP	1.54e-11	2.90e-12	-0.99		31	CCO-O2. + CCO-O2. = #2 {C-O2. + CO2} + O2
PPN2	1.20e-11	1.20e-11	0.00	-0.9	56,57	RCO-O2. + NO2 = PAN2
PAN2	5.87e-4	2.00e+15	25.44		57,58	PAN2 = RCO-O2. + NO2
PPNO	Same k as rxn APNO				59,57	RCO-O2. + NO = NO2 + CCHO + RO2-R. + CO2
PPH2	Same k as rxn APH2				59,57	RCO-O2. + HO2. = RCO-OOH + O2
PPN3	Same k as rxn APN3				59,57	RCO-O2. + NO3 = NO2 + CCHO + RO2-R. + CO2 + O2
PPME	Same k as rxn APME				59,57	RCO-O2. + C-O2. = RCO-OH + HCHO + O2
PPRR	Same k as rxn APRR				59,57	RCO-O2. + RO2-R. = RCO-OH + O2
PPR2	Same k as rxn APRR				59,43	RCO-O2. + R2O2. = RCO-O2.
PPRN	Same k as rxn APRR				59,46,57	RCO-O2. + RO2-N. = RCO-OH + PROD2 + O2
PPAP	Same k as rxn APAP				59,57	RCO-O2. + CCO-O2. = #2 CO2 + C-O2. + CCHO + RO2-R. + O2
PPPP	Same k as rxn APAP				59,57	RCO-O2. + RCO-O2. = #2 {CCHO + RO2-R. + CO2}
BPN2	1.37e-11	1.37e-11			60	BZCO-O2. + NO2 = PBZN
BPAN	4.27e-4	7.90e+16	27.82		61	PBZN = BZCO-O2. + NO2
BPNO	Same k as rxn APNO				62,63	BZCO-O2. + NO = NO2 + CO2 + BZ-O. + R2O2.
BPH2	Same k as rxn APH2				62,63	BZCO-O2. + HO2. = RCO-OOH + O2 + #4 XC
BPN3	Same k as rxn APN3				62,63	BZCO-O2. + NO3 = NO2 + CO2 + BZ-O. + R2O2. + O2
BPME	Same k as rxn APME				62,63	BZCO-O2. + C-O2. = RCO-OH + HCHO + O2 + #4 XC
BPRR	Same k as rxn APRR				62,63	BZCO-O2. + RO2-R. = RCO-OH + O2 + #4 XC
BPR2	Same k as rxn APRR				43,62	BZCO-O2. + R2O2. = BZCO-O2.
BPRN	Same k as rxn APRR				46,62,63	BZCO-O2. + RO2-N. = RCO-OH + PROD2 + O2 + #4 XC
BPAP	Same k as rxn APAP				62,63	BZCO-O2. + CCO-O2. = #2 CO2 + C-O2. + BZ-O. + R2O2.
BPPP	Same k as rxn APAP				62,57,63	BZCO-O2. + RCO-O2. = #2 CO2 + CCHO + RO2-R. + BZ-O. + R2O2.

Table 2. Listing and documentation of the reactions in the base mechanism.

Label	Rate Parameters [a] k(300)	A	Ea	B	Refs & Notes	Reaction and Products [b]
BPBP	Same k as rxn APAP				62,63	BZCO-O2. + BZCO-O2. = #2 {BZ-O. + R2O2. + CO2}
MPN2	Same k as rxn PPN2				62,64	MA-RCO3. + NO2 = MA-PAN
MPPN	4.79e-4	1.60e+16	26.80		65	MA-PAN = MA-RCO3. + NO2
MPNO	Same k as rxn APNO				62,64	MA-RCO3. + NO = NO2 + CO2 + HCHO + CCO-O2.
MPH2	Same k as rxn APH2				62,64	MA-RCO3. + HO2. = RCO-OOH + O2 + XC
MPN3	Same k as rxn APN3				62,64	MA-RCO3. + NO3 = NO2 + CO2 + HCHO + CCO-O2. + O2
MPME	Same k as rxn APME				62,64	MA-RCO3. + C-O2. = RCO-OH + HCHO + XC + O2
MPRR	Same k as rxn APRR				62,64	MA-RCO3. + RO2-R. = RCO-OH + XC
MPR2	Same k as rxn APRR				43,62	MA-RCO3. + R2O2. = MA-RCO3.
MPRN	Same k as rxn APRR				62,64	MA-RCO3. + RO2-N. = #2 RCO-OH + O2 + #4 XC
MPAP	Same k as rxn APAP				62,64	MA-RCO3. + CCO-O2. = #2 CO2 + C-O2. + HCHO + CCO-O2. + O2
MPPP	Same k as rxn APAP				62,64	MA-RCO3. + RCO-O2. = HCHO + CCO-O2. + CCHO + RO2-R. + #2 CO2
MPBP	Same k as rxn APAP				62,64	MA-RCO3. + BZCO-O2. = HCHO + CCO-O2. + BZ-O. + R2O2. + #2 CO2
MPMP	Same k as rxn APAP				62,64	MA-RCO3. + MA-RCO3. = #2 {HCHO + CCO-O2. + CO2}
Other Organic Radical Species						
TBON	2.40e-11	2.40e-11			66,67	TBU-O. + NO2 = RNO3 + #-2 XC
TBOD	1.18e+3	7.50e+14	16.20		68,67	TBU-O. = ACET + C-O2.
BRN2	3.79e-11	2.30e-11	-0.30		69	BZ-O. + NO2 = NPHE
BRH2	Same k as rxn RRH2				70	BZ-O. + HO2. = PHEN
BRXX	1.00e-3	1.00e-3			71	BZ-O. = PHEN
BNN2	Same k as rxn BRN2				72	BZ(NO2)-O. + NO2 = #2 XN + #6 XC
BNH2	Same k as rxn RRH2				70	BZ(NO2)-O. + HO2. = NPHE
BNXX	Same k as rxn BRXX				71	BZ(NO2)-O. = NPHE
Explicit and Lumped Molecule Organic Products						
FAHV	Phot Set= HCHO_R				73	HCHO + HV = #2 HO2. + CO
FAVS	Phot Set= HCHO_M				73	HCHO + HV = H2 + CO
FAOH	9.19e-12	8.60e-12	-0.04		31	HCHO + HO. = HO2. + CO + H2O
FAH2	7.79e-14	9.70e-15	-1.24		31	HCHO + HO2. = HOCOO.
FAHR	1.76e+2	2.40e+12	13.91		31	HOCOO. = HO2. + HCHO
FAHN	Same k as rxn MER1				74	HOCOO. + NO = HCOOH + NO2 + HO2.
FAN3	6.06e-16	2.00e-12	4.83		75	HCHO + NO3 = HNO3 + HO2. + CO
AAOH	1.57e-11	5.60e-12	-0.62		31	CCHO + HO. = CCO-O2. + H2O
AAHV	Phot Set= CCHO_R				76	CCHO + HV = CO + HO2. + C-O2.
AAN3	2.84e-15	1.40e-12	3.70		77	CCHO + NO3 = HNO3 + CCO-O2.
PAOH	2.00e-11	2.00e-11			78,31,79,80	RCHO + HO. = #.034 RO2-R. + #.001 RO2-N. + #.965 RCO-O2. + #.034 CO + #.034 CCHO + #-0.003 XC
PAHV	Phot Set= C2CHO				78,76	RCHO + HV = CCHO + RO2-R. + CO + HO2.

Table 2. Listing and documentation of the reactions in the base mechanism.

Label	Rate Parameters [a] k(300)	A	Ea	B	Refs & Notes	Reaction and Products [b]
PAN3	Same k as rxn AAN3				78,81	RCHO + NO3 = HNO3 + RCO-O2.
K3OH	1.94e-13	1.10e-12	1.03		31,82	ACET + HO. = HCHO + CCO-O2. + R2O2.
K3HV	Phot Set= ACETONE				83	ACET + HV = CCO-O2. + C-O2.
K4OH	1.20e-12	1.30e-12	0.05	2.0	31,79,80	MEK + HO. = #.37 RO2-R. + #.042 RO2-N. + #.616 R2O2. + #.492 CCO-O2. + #.096 RCO-O2. + #.115 HCHO + #.482 CCHO + #.37 RCHO + #.287 XC
K4HV	Phot Set= KETONE, qy= 1.0e-1				84	MEK + HV = CCO-O2. + CCHO + RO2-R.
MeOH	9.34e-13	3.10e-12	0.72	2.0	85	MEOH + HO. = HCHO + HO2.
MER9	5.46e-12	2.90e-12	-0.38		86	COOH + HO. = H2O + #.35 {HCHO + HO.} + #.65 C-O2.
MERA	Phot Set= COOH				87	COOH + HV = HCHO + HO2. + HO.
LPR9	1.10e-11	1.10e-11			88,89	ROOH + HO. = H2O + RCHO + #.34 RO2-R. + #.66 HO.
LPRA	Phot Set= COOH				90	ROOH + HV = RCHO + HO2. + HO.
GLHV	Phot Set= GLY_R				91,92	GLY + HV = #2 {CO + HO2.}
GLVM	Phot Set= GLY_ABS, qy= 6.0e-3				91,93	GLY + HV = HCHO + CO
GLOH	1.10e-11	1.10e-11			31,94,95	GLY + HO. = #.63 HO2. + #1.26 CO + #.37 RCO-O2. + #-.37 XC
GLN3	Same k as rxn AAN3				95,96	GLY + NO3 = HNO3 + #.63 HO2. + #1.26 CO + #.37 RCO-O2. + #-.37 XC
MGHV	Phot Set= MGLY_ADJ				97	MGLY + HV = HO2. + CO + CCO-O2.
MGOH	1.50e-11	1.50e-11			31	MGLY + HO. = CO + CCO-O2.
MGN3	Same k as rxn AAN3				96	MGLY + NO3 = HNO3 + CO + CCO-O2.
BAHV	Phot Set= BACL_ADJ				91,98	BACL + HV = #2 CCO-O2.
PHOH	2.63e-11	2.63e-11			99,100	PHEN + HO. = #.24 BZ-O. + #.76 RO2-R. + #.23 GLY + #4.1 XC
PHN3	3.78e-12	3.78e-12			99,101	PHEN + NO3 = HNO3 + BZ-O.
CROH	4.20e-11	4.20e-11			99,102	CRES + HO. = #.24 BZ-O. + #.76 RO2-R. + #.23 MGLY + #4.87 XC
CRN3	1.37e-11	1.37e-11			99,101	CRES + NO3 = HNO3 + BZ-O. + XC
NPN3	Same k as rxn PHN3				103	NPHE + NO3 = HNO3 + BZ(NO2)-O.
BZOH	1.29e-11	1.29e-11			99	BALD + HO. = BZCO-O2.
BZHV	Phot Set= BZCHO, qy= 5.0e-2				104	BALD + HV = #7 XC
BZNT	2.73e-15	1.40e-12	3.72		105	BALD + NO3 = HNO3 + BZCO-O2.
MAOH	3.35e-11	1.86e-11	-0.35		106,80,107	METHACRO + HO. = #.5 RO2-R. + #.416 CO + #.084 HCHO + #.416 MEK + #.084 MGLY + #.5 MA-RCO3. + #-0.416 XC
MAO3	1.19e-18	1.36e-15	4.20		106,108, 109,110	METHACRO + O3 = #.008 HO2. + #.1 RO2-R. + #.208 HO. + #.1 RCO-O2. + #.45 CO + #.117 CO2 + #.2 HCHO + #.9 MGLY + #.333 HCOOH + #-0.1 XC

Table 2. Listing and documentation of the reactions in the base mechanism.

Label	Rate Parameters [a]				Refs & Notes	Reaction and Products [b]
	k(300)	A	Ea	B		
MAN3	4.76e-15	1.50e-12	3.43		106,111, 80,112	METHACRO + NO3 = #.5 {HNO3 + RO2-R. + CO +MA-RCO3.} + #1.5 XC + #.5 XN
MAOP	6.34e-12	6.34e-12			113,5	METHACRO + O3P = RCHO + XC
MAHV	Phot Set= ACROLEIN, qy= 4.1e-3				106,114	METHACRO + HV = #.34 HO2. + #.33 RO2-R. + #.33 HO. + #.67 CCO-O2. + #.67 CO + #.67 HCHO + #.33 MA-RCO3. + #-0 XC
MVOH	1.87e-11	4.14e-12	-0.90		106,80	MVK + HO. = #.3 RO2-R. + #.025 RO2-N. + #.675 R2O2. + #.675 CCO-O2. + #.3 HCHO + #.675 RCHO + #.3 MGLY + #-0.725 XC
MVO3	4.74e-18	7.51e-16	3.02		106,108, 109,80, 110	MVK + O3 = #.064 HO2. + #.05 RO2-R. + #.164 HO. + #.05 RCO-O2. + #.475 CO + #.124 CO2 + #.1 HCHO + #.95 MGLY + #.351 HCOOH + #-0.05 XC
MVN3		(Slow)			106	MVK + NO3 = #4 XC + XN
MVOP	4.32e-12	4.32e-12			113,5	MVK + O3P = #.45 RCHO + #.55 MEK + #.45 XC
MVHV	Phot Set= ACROLEIN, qy= 2.1e-3				106,114, 115	MVK + HV = #.3 C-O2. + #.7 CO + #.7 PROD2 + #.3 MA-RCO3. + #-2.4 XC
IPOH	6.19e-11	6.19e-11			116,106, 80	ISOPROD + HO. = #.705 RO2-R. + #.006 RO2-N. + #.0 R2O2. + #.289 MA-RCO3. + #.357 CO + #.056 HCHO + #.134 CCHO + #.015 RCHO + #.158 MEK + #.352 PROD2 + #.158 GLY + #.179 MGLY + #-0.514 XC
IPO3	4.18e-18	4.18e-18			116,106, 80,117, 109,118, 110	ISOPROD + O3 = #.4 HO2. + #.048 RO2-R. + #.048 RCO-O2. + #.285 HO. + #.498 CO + #.14 CO2 + #.125 HCHO + #.047 CCHO + #.21 MEK + #.023 GLY + #.742 MGLY + #.1 HCOOH + #.372 RCO-OH + #-.33 XC
IPN3	1.00e-13	1.00e-13			116,106, 80	ISOPROD + NO3 = #.85 RO2-R. + #.15 MA-RCO3. + #.609 CO + #.15 HNO3 + #.241 HCHO + #.233 RCHO + #.008 MGLY + #.609 RNO3 + #.241 XN + #-.827 XC
IPHV	Phot Set= ACROLEIN, qy= 4.1e-3				116,106, 80,119	ISOPROD + HV = #1.233 HO2. + #.467 CCO-O2. + #.3 RCO-O2. + #1.233 CO + #.3 HCHO + #.467 CCHO + #.233 MEK + #-.233 XC
Lumped Parameter Organic Products						
K6OH	1.60e-11	1.60e-11			120	PROD2 + HO. = #.373 HO2. + #.479 RO2-R. + #.068 RO2-N. + #.028 CCO-O2. + #.052 RCO-O2. + #.218 HCHO + #.083 CCHO + #.555 RCHO + #.122 MEK + #.329 PROD2 + #.872 XC
K6HV	Phot Set= KETONE, qy= 1.0e-1				120,121	PROD2 + HV = #.968 RO2-R. + #.032 RO2-N. + #.708 R2O2. + #.4 CCO-O2. + #.6 RCO-O2. + #.331 HCHO + #.233 CCHO + #.878 RCHO + #-.221 XC
RNOH	8.50e-12	8.50e-12			122	RNO3 + HO. = #.309 NO2 + #.076 HO2. + #.426 RO2-R. + #.19 RO2-N. + #.639 R2O2. + #.026 HCHO + #.146 CCHO + #.393 RCHO + #.032 ACET + #.143 MEK + #.138 PROD2 + #.218 RNO3 + #.473 XN + #.559 XC

Table 2. Listing and documentation of the reactions in the base mechanism.

Label	Rate Parameters [a]				Refs & Notes	Reaction and Products [b]
	k(300)	A	Ea	B		
RNHV	Phot Set= IC3ONO2				122,123	RNO3 + HV = NO2 + #.263 HO2. + #.641 RO2-R. + #.096 RO2-N. + #.192 R2O2. + #.392 HCHO + #.085 CCHO + #.403 RCHO + #.052 ACET + #.143 MEK + #.445 PROD2 + #.251 XC
Uncharacterized Reactive Aromatic Ring Fragmentation Products						
D1OH	5.00e-11	5.00e-11			124,125	DCB1 + HO. = RCHO + RO2-R. + CO
D1HV		(Slow)			124,126	DCB1 + HV = HO2. + #2 CO + RO2-R. + GLY + R2O2.
D1O3	2.00e-18	2.00e-18			124,127, 117	DCB1 + O3 = #1.5 HO2. + #.5 HO. + #1.5 CO + #.5 CO2 + GLY
D2OH	5.00e-11	5.00e-11			128,129	DCB2 + HO. = R2O2. + RCHO + CCO-O2.
D2HV	Phot Set= MGLY_ABS, qy= 3.7e-1				128,130	DCB2 + HV = RO2-R. + #.5 {CCO-O2. + HO2.} + CO + R2O2. + #.5 {GLY + MGLY + XC}
D3OH	5.00e-11	5.00e-11			128,129	DCB3 + HO. = R2O2. + RCHO + CCO-O2.
D3HV	Phot Set= ACROLEIN, qy= 7.3e+0				128,130	DCB3 + HV = RO2-R. + #.5 {CCO-O2. + HO2.} + CO + R2O2. + #.5 {GLY + MGLY + XC}
Explicit Primary Organics						
c1OH	6.62e-15	2.15e-12	3.45		31	CH4 + HO. = H2O + C-O2.
ISOH	9.73e-11	2.50e-11	-0.81		131,132	ISOPRENE + HO. = #.909 RO2-R. + #.091 RO2-N. + #.079 R2O2. + #.626 HCHO + #.23 METHACRO + #.32 MVK + #.359 ISOPROD + #-.167 XC
ISO3	1.34e-17	7.86e-15	3.80		131,108, 133,110	ISOPRENE + O3 = #.066 RO2-R. + #.134 R2O2. + #.266 HO. + #.275 CO + #.122 CO2 + #.6 HCHO + #.1 PROD2 + #.39 METHACRO + #.16 MVK + #.2 MA-RCO3. + #.204 HCOOH + #.15 RCO-OH + #-.251 XC
ISN3	6.81e-13	3.03e-12	0.89		131, 134	ISOPRENE + NO3 = #.19 NO2 + #.76 RO2-R. + #.05 RO2-N. + #.19 R2O2. + #.95 ISOPROD + #-.05 XC + #.81 XN
ISOP	3.60e-11	3.60e-11			131,135	ISOPRENE + O3P = #.25 RO2-R. + #.25 R2O2. + #.5 HCHO + #.75 PROD2 + #.25 MA-RCO3. + #-1 XC

Footnotes for Table 2.

No.	Note
1	See Table ?? for listing of absorption cross sections and quantum yields. Set used is given in the "Type" column.
2	Absorption cross sections and quantum yields from IUPAC recommendation (Atkinson et al, 1997a), except that quantum yields for wl > 410 nm are from NASA (1997), which are consistent with IUPAC (Atkinson et al, 1997a) values except they are more precise. Note that more recent IUPAC recommendations (Atkinson et al, 1997b) gives slightly different absorption cross sections based on data from a more recent study, but the differences are not significant.
3	Rate constant expression derived from IUPAC (Atkinson et al, 1997b) recommendations for M = 20.9% O2 and 79.1% N2.
4	Rate constant is IUPAC, Supplement VI (Atkinson et al, 1997b) and NASA (1997) recommendation.
5	This reaction is probably not important in air, but is included to increase range of applicability
6	Rate constant expression is IUPAC (Atkinson et al, 1997b) recommendation.
7	Recommended rate constant given for N2 is assumed to be applicable to air.
8	The data of Mentel et al (1996) indicate that the reaction occurs through pathways which are first order and second order in H2O, where the latter is presumed to be surface-dependent. We assume that the process which is first order in H2O represents a gas-phase reaction, and use the rate expression of Mentel et al (1996) for this process. Note that the IUPAC (Atkinson et al, 1997b) recommendation that the gas-phase rate constant is less than 2×10^{-21} cm-3 molec-1 s-1.
9	Photolysis of N2O5 is assumed to be negligible compare to decomposition under atmospheric conditions.
10	The NASA (1997) evaluation states that the existence of this channel has not been firmly established, but results of a number of studies indicate it may occur. Rate constant expression used is that NASA (1997) states gives best fits to the data. Uncertainty is at least a factor of 2. This reaction was not discussed in the recent IUPAC evaluations (Atkinson et al, 1997a,b).
11	Absorption cross sections from IUPAC (Atkinson et al, 1997a). Values recommended by more recent IUPAC evaluation (Atkinson et al, 1997b) appear to be the same for 298K, though different at lower temperature. Temperature dependence ignored.
12	IUPAC (1997b) and NASA (1997) give no useable recommendations for quantum yields except to recommend that qy(NO2+O)=1 for wl <= 583. Quantum yields of Magnotta and Johnsom (1980), scaled down by a factor of 1.5 to give unit maximum quantum yields, as incorporated in mechanism of Carter (1990) were retained in this mechanism. The calculated rate constant for solar overhead sun is consistent with the recommendations of Magnotta and Johnson (1980), and reasonably consistent with the IUPAC (1997a) recommendation.
13	Absorption cross sections from IUPAC (Atkinson et al, 1997b). Data are for T=273 K. Temperature dependences for cross section (NASA, 1997) are ignored.
14	Quantum yields for O1D are those tabulated by IUPAC (Atkinson et al, 1997b), which are significantly higher than previous recommendations at wl > 310 nm. Quantum yields for O3P based on assuming total quantum yield of unity, though this was not adequately discussed in the evaluations.
15	Calculated using IUPAC (Atkinson et al, 1997b) recommended rate constants for reaction with O2 and N2, assuming 20.9% O2 and 79.1% N2. Temperature dependence optimized to fit rate constants calculated for T= 270, 300, and 330K.
16	Falloff expression recommended by NASA (1997) used because it gives rate constant for 1 atm N2 which is consistent with measurement near those conditions. IUPAC (Atkinson et al, 1997a,b) recommendations are not used because k (1 atm N2) are not consistent with these data, being based on high pressure data in He. This is consistent with current recommendation of Atkinson (private communication, 1997).
17	The cross sections from Stockwell and Calvert (1978), used in the previous version of the mechanism, are retained because they are higher resolution than the averaged data recommended by IUPAC (1997b), and the areas under the spectra appear to be consistent.

Footnotes for Table 2.

No.	Note
18	Quantum yields are those recommended by IUPAC (Atkinson et al, 1997b).
19	NASA (1997) and IUPAC (Atkinson et al, 1997a,b) give significantly different recommendations for rate parameters for this important reaction. The falloff expression used here is based on a NASA (1997) and IUPAC (Atkinson et al, 1997a,b) give significantly different recommendations for rate parameters for this important reaction. The falloff expression used here is based on a re-evaluation of the data by Golden (Personal communication, 1998), and is expected to be the recommendation in the next NASA evaluation. This is essentially the same as the NASA (1997) recommendation except for the temperature dependence, which Golden says was due to improper uncertainty weighting. The data with "weak colliders (i.e., bath gases other than SF6 or CF4) appear to be well fit by this parameterization, including the data of Donahue et al (1997). The data of Forster et al (1995), which are the basis for the high 1997 IUPAC recommendation, are not used because they may be due to a HOONO-forming channel becoming important at high pressure.
20	No recommendation is given concerning the temperature dependence of this rate constant, which is assumed to be small.
21	The rate parameters were derived to fit the rate constants calculated using the NASA (1997) recommended expression for T 270 - 330 K range and 1 atm. total pressure
22	This rate constant is strictly valid for 1 atm air only, but the error introduced by neglecting the pressure dependence of this reaction is expected to be small.
23	Absorption cross-sections from IUPAC (Atkinson et al, 1997b). Recommend quantum yield for the OH + NO2 pathway is "close to unity" for wl > 260 nm, though other pathways become important at lower wavelengths.
24	The rate constants for the OH + CO reactions are based on expression given by IUPAC (Atkinson et al, 1997a). NASA (1997) gives a similar expression, but without temperature dependence.
25	Absorption cross sections and quantum yields from IUPAC (Atkinson et al, 1997b). Quantum yields are uncertain and based on data for a single wavelength only.
26	Reactions and rate constants used for the HO2 + HO2 and HO2 + HO2 + H2O system based on the data of Kircher and Sander (1984) as discussed in the IUPAC (Atkinson et al, 1997b) evaluation.
27	Rate constant recommended by IUPAC (Atkinson et al, 1997b). Mechanism based on data of Mellouki et al (1993) as discussed by IUPAC (Atkinson et al, 1997b).
28	Rate expression from NASA (1994) evaluation. More recent evaluations neglect this reaction, though it may be non-negligible under some nighttime conditions (Stockwell et al, 1997).
29	Absorption cross sections recommended by IUPAC (Atkinson et al, 1997a,b) used. Quantum yield assumed to be unity.
30	The initially formed $HOSO_2$ is assumed to react primarily with O_2, forming HO2 and SO_3. The SO_3 is assumed to be converted into sulfates, which are represented by the SULF model species.
31	Rate constant expression recommended by IUPAC, Supplement VII (Atkinson et al, 1999).
32	The reaction of NO2 is ignored because it is rapidly reversed by the decomposition of the peroxynitrate, resulting in no net reaction. Calculations not neglecting peroxynitrate formation give essentially the same results. However, this may not be valid in low temperature simulations.
33	Total rate constant and rate constant for methoxy radical formation from IUPAC (Atkinson et al, 1997a, 1999) recommendation. Temperature dependence for rate constant for methanol + HCHO formation derived to be consistent with these.
34	The RO2-R. operator represents the effects of peroxy radicals which react with NO to form NO2 and HO2, and also the effects of peroxy radical reactions on other species. Except as indicated, the organic products from this peroxy radical are not represented.
35	Rate constant recommended by Atkinson (1997a) for general peroxy radicals.
36	The organic products from the HO2 reaction are represented by the lumped higher hydroperoxide species. Negative "lost carbons" are added because this is a zero-carbon operator.

Footnotes for Table 2.

No.	Note
37	Rate constant based on that recommenced by IUPAC (Atkinson et al, 1999) for ethyl peroxy + NO3. Formation of alkoxy + NO2 + O2 stated to occur >85% of the time.
38	The reaction is assumed to form the corresponding alkoxy radical. The HO2 represents the radicals regenerated by the alkoxy radical.
39	Based on rate constant for methyl peroxy + ethyl peroxy rate given by Atkinson (1997a). This is near the middle of the range of rate constants given for other methyl peroxy + higher alkyl peroxy radical reactions given by Atkinson (1997a) or Atkinson et al (1997a).
40	Approximately half of the peroxy + peroxy reaction is assumed to form two O2 + alkoxy radicals. The HO2 represents the radicals regenerated in the fraction of this peroxy radical which reacts in this way.
41	The rate constants for peroxy + peroxy radical reactions can vary by orders of magnitude depending on the type of radical (e.g., Atkinson, 1997), so the value used here must be approximate. Value used is based roughly on range of rate constants for secondary peroxy radicals as given by Atkinson (1997a).
42	Assumed to have same rate constant as used for general higher peroxy radical (see notes for RO2-R.).
43	The R2O2. operator represents the effects of peroxy radical reactions causing extra NO to NO2 conversions. Its reactions with species other than NO are represented as having no effect other than to consume this operator.
44	The RO2-N. operator represents the effects of peroxy radicals which react with NO to form higher organic nitrates (represented by RNO3), and also the effects of peroxy radical reactions on other species. It has five carbons.
45	The organic products from the HO2 reaction are represented by the lumped higher hydroperoxide species. "Lost carbons" are added because this is a five-carbon operator.
46	Approximately half of the peroxy + peroxy reaction for radicals represented by RO2-N. is assumed to form two O2 + alkoxy radicals. The MEK + HO2. represents the products and radicals formed from the alkoxy radical from this species. The other half is assumed to involve disproportionation, forming O2 + and an alcohol and carbonyl compound. These are represented by PROD2.
47	This reaction is assumed to form the corresponding alkoxy radical, which is assumed to react products represented by MEK + HO2.
48	Falloff expression recommended by IUPAC (Atkinson et al, 1997a, 1999), based on data of Bridier et al (1991).
49	Falloff expression recommended by IUPAC (Atkinson et al, 1992), based on data of Bridier et al (1991). Note: NASA (1997) also recommends using Bridier et al (1991) data, but gives a revised expression which gives a different k at 298K. Based on new data on PAN decomposition which give a factor of ~2 lower rate 298K rate constants, IUPAC (1997a, 1999) recommends the a high pressure rate constant expression of 5.4×10^{16} exp(-13830/T), derived by averaging the data. We are staying with the earlier IUPAC Recommendations based on the data of Bridier et al (1991) because it gives good agreement with the data of Tuazon et al (1991) and is consistent with the NASA (1997) recommended equilibrium constant.
50	Rate constant based on the IUPAC (Atkinson et al, 1997a) recommendation is to use k(NO)/K(NO2)=2.1 for atmospheric conditions (298K and 1 atm.), with k(NO) approximately independent of temperature. This is almost the same as the IUPAC(Atkinson et al, 1997a, 1999) recommended value of 2.0×10^{11} and the NASA (1997) value of 1.8×10^{-11}.
51	Branching ratio and rate constant expression recommended by IUPAC (Atkinson et al, 1997a, 1999).
52	Rate constant from Canosa-Mass et al (1996)
53	Rate constant expression recommended by IUPAC (Atkinson et al, 1999) evaluation. As discussed there, the data are inconclusive as to the importance of the competing reaction forming CH3O + CH3CO2 + O2, but the study which indicate that it occurs, which was used in the previous IUPAC (Atkinson et al, 1997a) evaluation, indicates that it occurs less than ~15% under atmospheric conditions. Therefore, the reaction is assumed to involve disproportionation 100% of the time.

Footnotes for Table 2.

No.	Note
54	Rate constant based on values for rate constants for acetyl peroxy + methyl peroxy and $CH_3C(O)CH_200$. given by Atkinson et al (1997a).
55	This reaction is assumed to proceed primarily by disproportionation to form the organic acid and a carbonyl compound, based on data for the acetyl peroxy + methyl peroxy reaction.
56	The rate parameters are assumed to be approximately the same as those for the reaction of CH3C(O)OO. at the high pressure limit. NASA (1997) and IUPAC (Atkinson et al, 1997a, 1999) give no recommendations for this rate constant for higher acyl peroxy radicals.
57	The products of the reactions of RCO-O2. are based on R=ethyl. Mechanism assumed to be similar to corresponding reaction of acetyl peroxy radicals.
58	Rate parameters based on data for PPN. The activation energy is recommended by Atkinson (1994) for thermal decomposition of higher PAN analogues. The A factor is adjusted to yield the average k(298) for PPN as measured by Schurath and Wipprecth (1980) and Mineshos and Glavas (1991). The A factor recommended by Atkinson (1994) not used because it gives k(298) outside the range of both those measurements.
59	Assumed to have same rate constant as corresponding reaction of $CH_3C(O)OO$.
60	Rate constant based on $k(NO_2)/k(NO)$ ratio measured by Kirchner et al (1992) and the k(NO) used for general higher acyl peroxy radical species.
61	Rate constant expression based on the data of Kirchner et al (1992).
62	Assumed to have the same rate constant and mechanism as used for the general higher acyl peroxy radical or higher PAN analogue
63	The mechanism is assumed to be analogous to the mechanism of the corresponding reaction of acetyl peroxy radicals. Note that the formation of benzyl peroxy radicals results in the formation of phenoxy after 1 NO to NO2 conversion, so it can be represented by BZ-O. + R2O2. The general lumped higher orgainc acid (RCO-OH) and peroxyacid (RCO-OOH) are used to represent the aromatic acids and peroxyacids expected to be formed in the peroxy + peroxy reactions.
64	MA-RCO3. And MA-PAN are used to represent the acyl peroxy radical and PAN analogue formed from any acrolein compound. Their reactions are are based on those formed from methacrolein. Generally, the reaction mechanisms are assumed to be analogous to those for the corresponding reactions of acetyl peroxy radicals. The alkoxy radical is assumed to decompose to CO2 + CH2=CH(.)CH3, while the latter reacts with O2 to form HCHO + CH3CO., as discussed by Carter and Atkinson (1996). The general lumped higher orgainc acid (RCO-OH) and peroxyacid (RCO-OOH) are used to represent the unsaturated acids and peroxyacids expected to be formed in the peroxy + peroxy reactions.
65	Rate parameters from Roberts and Bertman (1992), as used by Carter and Atkinson (1996)
66	The rate expression recommended by Atkinson (1997) for general alkoxy + NO_2 reactions is $2.3x10^{-11}$ exp(+150/T). This is reduced by a factor of 1.58 to be consistent with environmental chamber data, as discussed in a separate note.
67	The effects of isobutane and t-butyl alcohol on ozone formation and radical levels in environmental chamber experiments are not consistent with predictions of models which assume the recommended rate constant ratios for the decomposition of t-butoxy radicals relative to reaction with NO_2. The data are better fit if the ratio is increased by a factor of 2.5. The error is assumed to be equally distributed in each rate constant, so they are both adjusted by the a factor of 1.58, which is the square root of 2.5
68	Atkinson (1997b) recommends the high-pressure rate expression of 6.0x10+14 exp(-16.2/RT). Batt and Robinson (1987) calculate that at one atmosphere the rate constant is 79% the high pressure limit, giving an estimated rate expression of 4.74x10-14 exp(-16.2/RT). This is increased by a factor of 1.58 to be consistent with environmental chamber data, as discussed in a separate note.

Footnotes for Table 2.

No.	Note
69	The rate constant is based on the general recommendation of Atkinson (1994) for alkoxy + NO2 reactions at the high pressure limit. Nitrophenol formation has generally been assumed in this reaction (e.g., see Atkinson, 1990; Carter, 1990), presumably via some rearrangement of an initially-formed unstable adduct. However, based on lower than expected yields of nitrophenols in NO3 + cresol and OH + benzaldehyde systems (Atkinson, 1994), this may be an oversimplification.
70	Assumed to have the same rate constant as the reaction of HO2 with peroxy radicals. This may underestimate the actual rate constant.
71	This is included to avoid problems if these radicals are ever formed under conditions where both HO_2 and NO_2 are very low (which is considered to be unlikely under most ambient conditions), and can be considered to represent its reaction with organics present. The rate constant is arbitrary, and is such that this process becomes significant only if $[NO_2] < \sim 3x10^{-6}$ ppm and $[HO_2] < 1x10^{-5}$ ppm.
72	The rate constant is based on the general recommendation of Atkinson (1994) for alkoxy + NO2 reactions at the high pressure limit. The products of this reaction (presumed to be aromatic dinitro compounds) are expected to have very low vapor pressures and are represented as unreactive nitrogen and carbon.
73	Absorption cross sections and quantum yields recommended by IUPAC (Atkinson et al, 1997a) used. Absorption cross sections used are those given for T = 285K.
74	Rate constant assumed to be the same as used for methylperoxy + NO
75	T=298K Rate constant recommended by IUPAC (Atkinson et al, 1979a). Temperature dependence is as estimated by IUPAC (Atkinson et al, 1979a).
76	Absorption cross sections and quantum yields recommended by IUPAC (Atkinson et al, 1997a, 1999) used. Reaction assumed to occur primarily by breaking the C-CHO bond. Pathway forming molecular products from acetaldehyde is calculated to be negligible under atmospheric conditions, and is not included in the model.
77	Rate constant expression recommended by IUPAC, Supplement V (Atkinson et al, 1997a)
78	The mechanism for RCHO is based on reactions estimated for propionaldehyde.
79	OH reactions at various positions in the molecule estimated using the group-additivity methods of Kwok and Atkinson (1995), as updated by Kwok et al (1996).
80	Except as indicated by other footnotes, the overall reaction mechanism was derived using the general estimation methods for atmospheric reactions of alkyl, alkyl peroxy, and alkoxy radicals and the automated mechanism generation system as discussed by Carter (1999).
81	Assumed to have same rate constant and analogous mechanism as reaction of acetaldehyde.
82	Reaction in the presence of NOx is assumed to involve formation of $CH_3C(O)CH2O.$, after one NO to NO2 conversion. Based on the data of Jenkin et al (1993), this radical is believed to rapidly decompose to HCHO + CH3CO.
83	Absorption cross sections and quantum yields used are those recommended by IUPAC (Atkinson et al, 1997a) except as noted. The reported quantum yields at 230 and 330 are expected to be high and an estimated correction was made as discussed by Carter et al (1993b). The corrected quantum yield data for wavelengths less than 290 nm were then fit to a smooth curve to estimate the quantum yields for higher wavelengths, with no weight being given to the highly uncertain 330 nm point. As discussed by Carter et al (1993b), using these corrections results in better fits of model calculations to environmental chamber experiments involving acetone.
84	The absorption coefficients used for MEK are from Moortgat (Private communication, 1996). The overall MEK quantum yield of 0.1 was derived from fits to UNC chamber data as determined by Carter et al (1986), and is consistent with results of MEK reactivity experiments carried out in our laboratories (Carter et al, 1999a). The reaction is assumed to proceed primarily by breaking the weakest CO-C bond.

Footnotes for Table 2.

No.	Note
85	The mechanism and rate constants are as recommended by IUPAC (Atkinson et al, 1997a, 1999). The branching ratio is for T=298K only. The overall reaction assumes the major fate of the alpha hydorxy radical is reaction with O_2 to form HO_2 and HCHO.
86	Rate constant and branching ratio for initial OH reaction based on IUPAC (Atkinson et al, 1997a, 1999) recommendation. The .CH2OOH radical is assumed to rapidly decompose to HCHO + OH, based on its high estimated exothermicity.
87	Absorption cross sections from IUPAC (Atkinson et al, 1997a, 1999), which also recommends assuming unit total quantum yield, but gives no recommendation as to the exact mechanism. Breaking the O-O bond assumed to be the major pathway.
88	The mechanism for ROOH is based on reactions estimated for n-propyl hydroperoxide.
89	Reaction at the OOH position is assumed to be as fast as in CH3OOH. Reaction at the 1-position is estimated to be ~7x10-12 (i.e., ~2/3 of the time) based on comparing rates of analogous reactions for methanol, ethanol, and CH3OOH (IUPAC, 1997a, 1999). The alpha-hydroperoxy radicals are assumed to decompose rapidly to OH and the carbonyl on the basis of estimated high exothermicity. Reaction at the 2- or 3-positions are estimated to occur no more than ~10% of the time and are neglected.
90	Reaction assumed to occur with the same rate and analogous mechanism as methyl hydroperoxide
91	Absorption cross sections from Plum et al (1983), as recommended by IUPAC (Atkinson et al, 1997a, 1999) in the case of glyoxal.
92	For the low wavelength band, a constant quantum yield of 0.4 is assumed, based on data of Langford and Moore (1984). For the high wavelength band, quantum yield is assumed to decrease linearly to zero at the threshold wavelength of 418 nm, starting at a "falloff" wavelength, which is adjusted to yield fits to chamber data for acetylene - NOx and acetylene reactivity experiments, as discussed by Carter et al (1997c). "Best fit" falloff wavelength of 380 nm used. Note that this gives overall quantum yields which are ~1.4 times higher than overall quantum yield reported by Plum et al (1983) for conditions of those experiments. Although use of acetylene reactivity data is a highly indirect way to obtain glyoxal quantum yields, it is considered to be a less uncertain way to estimate radical quantum yields then the data of Plum et al (1993), which uses a UV-poor light source and only measures rates of glyoxal decay.
93	Plum et al (1983) observed 13% formaldehyde yield in photodecomposition, so overall quantum yield adjusted to give this yield relative to the radical forming process for the spectral distribution of those experiments. A wavelength-independent quantum yield is used because of lack of information on wavelength dependence.
94	Product distribution based on the data of Niki et al (1985), as discussed by IUPAC (Atkinson et al, 1997a). Product distribution is calculated for 1 atm air at 298K
95	HCO(CO)OO. is represented by the lumped higher acyl peroxy species RCO-OO.
96	Assumed to have the same rate constant and mechanism as the analogous reaction with acetaldehyde.
97	Absorption cross sections obtained from Moortgat (personal communication, 1996). These are essentially the same as those recommended by IUPAC (Atkinson et al, 1997a, 1999), except slightly better resolution. Photolysis at the low wavelength band is assumed to have unit quantum yields, based on data for biacetyl. Photolysis above the cutoff wavelength of 421 nm (Atkinson et al, 1977a) is assumed to have zero quantum yields. For the rest of the high wavelength region, the wavelength dependence was derived by assuming the quantum yields decline linearly from 1 at 344 nm to 0 at a wavelength (407 nm) which was adjusted to be such that the calculated overall quantum yields for the conditions of the experiments of Plum et al (1983) agreed with the overall quantum yield they observed experimentally. The quantum yields recommended by IUPAC (Atkinson et al, 1999) lack sufficient wavelength resolution to be useful for modeling.

Footnotes for Table 2.

No.	Note
98	Assumed to have unit quantum yield at low wavelength band based on data cited by Atkinson (1994). For the high wavelength band, the quantum yields were assumed to decline linearly from 1 at 350 nm to 0 at a wavelength (420 nm) which was adjusted to be such that the calculated overall quantum yields for the conditions of the experiments of Plum et al (1983) agreed with the overall quantum yield they observed experimentally.
99	Rate constant recommended by Atkinson (1994).
100	The parameterized mechanism is estimated by analogy to the parameterized mechanism derived for cresols (see footnotes for OH + cresol reaction).
101	In absence of definitive data concerning this reaction, the same mechanism is used as assumed by Carter (1990). However, see footnotes concerning phenoxy reactions.
102	The parameterized mechanism is based on that used by Carter (1990), but was reoptimized to fit the NO, ozone, PAN, and cresol data in the o-cresol - NOx experiment EC281.
103	Assumed to have the same rate constant as the reaction of NO_3 with phenol. Reaction with NO_3 is assumed to dominate over reaction with OH radicals and other loss processes.
104	Absorption coefficients are from Majer et al (1969). The overall quantum yield derived by Carter (1990), which are based on model simulations of benzaldehyde decay rates in SAPRC evacuable chamber experiments, is used. Because of lack of data, the quantum yield is assumed to be independent of wavelength. The products formed from benzaldehyde photolysis are unknown, except that both radical formation and benzene formation appear to be minor (Carter, 1990). This benzaldehyde photolysis mechanism gives reasonably good model simulations of benzaldehyde - NOx experiments recently carried out in the CE-CERT xenon Teflon chamber (Carter et al, 1998a).
105	T=298K rate constant recommended by Atkinson (1994). Temperature dependence estimated by assuming the reaction has the same A factor as the reaction of NO_3 with acetaldehyde.
106	The rate constant and mechanism of Carter and Atkinson (1996) was used with no significant changes (except as indicated in other footnotes, if applicable). Some minor changes in product yields may result in some cases from use of the general mechanism estimation system (Carter, 1999a) to generate the overall reaction scheme.
107	MEK is used to represent hydroxyacetone.
108	The excited $HCHO_2$ biradical is assumed to react as recommended by Atkinson (1997) based on data for the O3 + ethene system, i.e., 37% stabilization, 12% decomposition to HCO + OH, 13% decomposition to CO_2 + H_2, and 38% decomposition to CO + H_2O. Note that this is different than used for this species when formed in the isoprene products mechanisms of Carter and Atkinson (1996) and Carter (1996).
109	The vibrationally excited $HCOC(CH_3)CO_2$ biradicals are assumed to rearrange and decompose to $HCOC(O)CH_2$. + OH, where the former forms HCOC(O). + HCHO after O2 addition and NO to NO_2 conversion. RCO-O2. is used to represent HCOC(O)OO. in this reaction. Vibrationally excited $CH_3C(O)CHO_2$ is assumed to rapidly convert to $HCOC(CH_3)CO_2$ as discussed by Carter and Atkinson (1996).
110	The organic acid(s) formed in this reaction represent the formation of stabilizied Crigiee biradicals, which are assumed to be consumed primairly by reaction with H_2O forming the corresponding acid.
111	NO_3 radical addition assumed to occur primarily at the least substituted position.
112	The product CH3C(O)CH2ONO2 is expected to be relatively unreactive and is represented as "lost nitrogen" + 3 "lost carbons".
113	Rate constant estimated from linear correlation between log k for OH and O3P reaction. Chamber data for C_{3+} alkenes are better fit by models assuming O3P reactions with C_{3+} species do not form radicals. Stable products represented by the lumped higher aldehyde or ketone, depending on type of product(s) expected to be formed.

Footnotes for Table 2.

No.	Note
114	The overall quantum yield was reoptomized to fit the same data as discussed by Carter and Atkinson (1996). In the case of methacrolein, he changes to the other portion of the mechanism resulted in an ~14% increase in the best fit overall quantum yield compared to that derived by Carter and Atkinson (1996). In the case of MVK, the best fit overall quantum yield decreased by a factor of 5.
115	CH_2=CHC(O)OO. Is represented by MA-RCO3.
116	As discussed by Carter (1996), isoprod is the "four product" lumped isoprene product species whose mechanism is derived by lumping rate constant and product parameters for a mixture of 30% hydroxymethacrolein, and 70% equal amounts of cis and trans $HCOC(CH_3)=CHCH_2OH$ and $HCOCH=C(CH_3)CH_2OH$. These proportions are based on the estimated yields of these products in the reactions of OH with isoprene (Carter and Atkinson, 1996), which are represented by ISOPROD in the four product condensed mechanism (Carter, 1996). The other footnotes refer to the estimated mechanisms for these four individual compounds which were used to derive the lumped ISOPROD mechanism. RCHO, PROD2, MA-RCO3, etc. are used to represent various compounds as indicated in the descriptions of these lumped model species. See Carter and Atkinson (1996) for the specific compounds which can be formed in the various reactions of these species.
117	The $HC(O)CHO_2$ biradical can decopose either to OH + HCO + CO via an internal H abstraction from HCO, or to HCO + HCO_2 via rearrangement to HCOCH(O.)O. and decomposition. (The HCO would form HO_2 + CO and the HCO_2 would form HO_2 + CO_2 after reaction with O_2.) These two pathways are assumed to have equal probability. Note that decomposition for these biradicals is assumed to be faster than for biradicals such as CH_3CHO_2 because of the weaker H-CO and C-CO bonds.
118	The excited $CH_3C(O_2)CH_2OH$ biradical is assumed to react primarily via rearrangement to the unsaturated hydroperoxide followed by decomposition to OH radicals and the corresponding carbonyl compound, as is assumed in the general alkene mechanism (Carter, 1999b). Two possible such rearrangements can occur in the case of this biradical, one to $CH_2=C(OOH)CH_2OH$, which decomposes to OH + $HOCH_2C(O)CH_2$., and the other to $HOCH=C(OOH)CH_3$, which decomposes to OH + $CH_3C(O)CH(.)OH$. The relative importances of the competing rearrangements in such cases is estimated by assuming they are approximately proportional to the estimated OH abstracting rate constant from the H-donating group (Carter, 1999b). Based on this, the overall reaction is estimated to be OH + 0.04 $HOCH_2C(O)CH_2$. + 0.96 $CH_3C(O)CH(.)OH$, with the subsequent reactions of these radicals being derived by the general estimation methods (Carter, 1999a).
119	All the species represented by ISOPROD are assumed to have the same overall photolysis rate as used for methacrolein.
120	The PROD2 mechanism was derived by averaging mechansims for $CH_3C(O)CH_2CH_2CH_2OH$, $CH_3C(O)CH_2CH(CH_3)CH_2OH$, $CH_3CH(OH)CH_2CH_2C(O)CH_2CH_3$, $CH_3CH_2CH(OH)CH_2CH2C(O)CH_2CH_3$, and $CH_3CH_2CH_2CH(OH)CH_2CH_2C(O)CH_2CH_3$, which were taken as representative of the products formed from VOCs measured in ambient air that are represented by PROD2 in the model (Carter, 1999). The mechansims for these five representative PROD2 compounds were derived using the mechanism generation and estimation methods discussed by Carter (1999).
121	Assumed to photolyze with the same rate absorption cross section and quantum yields as used for MEK.
122	The RNO3 mechanism was derived by averaging mechanisms for $CH_3CH_2CH_2CH_2CH(ONO_2)CH_2OH$, $CH_3CH(CH_3)CH_2C(CH_3)(ONO_2)CH_2CH_3$, and $CH_3CH_2CH(ONO_2)CH_2CH_2CH_2CH_3$, which were taken as representative of the products formed from VOCs measured in ambient air that are represented by RNO3 in the model (Carter, 1999). The mechanisms for these three representative RNO3 compounds were derived using the mechanism generation and estimation methods discussed by Carter (1999).

Footnotes for Table 2.

No.	Note
123	Absorption cross sections given by IUPAC (Atkinson et al, 1997a, 1999) for isopropyl nitrate are used. As discussed by IUPAC (Atkinson et al, 1999), the quantum yield is expected to be near unity for formation of NO2.
124	DCB1 is used to represent aromatic ring fragmentation products that do not undergo signficant photodecomposition to radicals. Its mechanism is largely parameterized, but it is based roughly on that expected for unsaturated dicarbonys such as 2-butene-1,3-dial.
125	The rate constant is based on data of Bierbach et al (1994). The reaction is assumed to proceed via addition of OH to double bond, followed by decomposition of the alkoxy radical to HCO and HC(O)CH(OH)CHO, where the latter is represented by RCHO. Although this mechanism may not be what one would estimate for the non-photoreactive unsaturated diketones (Bierback et al, 1994; Tuazon et al, ??) expected to be formed from o-substitued aromatics, best fits to the o-xylene and 1,2,4-trimethylbenzene chamber data are obtained if this mechanism is used.
126	The photolysis action spectra of these products are assumed to be similar to that for acrolein, so the absorption cross sections of acrolein are used, with a wavelength-independent overall quantum yield. The overall quantum yield is adjusted to optimize fits of model simulations to the benzene - NOx experiments used in the optimization of the previous version of the mechanism by Carter et al (1997a), The photolyisis mechanism is represented as being similar to that used for DCB2 and DCB3. However, best fits to benzene - NOx experiments are obtained if this photolysis is assumed to be slow, so the reaction is not included in the mechanism.
127	The rate constant is based on the data of Bierbach et al (1994). The reaction is assumed to involve initial formation of glyoxal and $HC(O)CHO_2$.
128	DCB2 and DCB3 represent the highly photoreactive unsaturated dicarbonyl product formed from the ring-opening reactions of the alkylbenzenes. To fit chamber data using differing light sources, they are represented by two species, which differ only in their action spectra and overall quantum yields, with the action spectrum of DCB2 being like methyl glyoxal, and that of DCB3 being like acrolein, and with the overall quantum yields adjusted separately to fit chamber data. Its reactions are based roughly on estimated reactions of a 5-carbon compound with general structure XC(O)CX=CXC(O)X, where X can be H or alkyl.
129	Assumed to have the same rate constant as used for DCB1. Mechanism represented as OH adding to double bond in XC(O)CX=CXC(O)X, with alkoxy radical decomposing to CH3CO. and XCO-CH(OH)-CXO, the latter being represented by RCHO. Note that the general alkoxy radical estimation method (Carter, 1999) predicts that alkoxy radicals like RCH(OH)CH(O.)C(O)R' will decompose primarily to RCH(OH)CHO + RC(O).
130	The overall quantum yields for DCB2 and DCB3 were optimized to give best fits of model simulations of NO oxidation, O3 formation and xylene consumption in m-xylene - NOx chamber runs with various light sources, and also to mini-surrogate - NOx runs. The DCB2 and DCB3 quantum yields had to be adjusted as well as the yields of these products from m-xylene to best fit the data for the various light sources, and also to fit the results of the mini-surrogate as well as the m-xylene only runs. (For the other aromatics, only the DCB2 and DCB3 yields are optimized.) The photolysis mechanisms are unknown, and probably highly variable depending on the species involved. For an RC(O)CH=CHC(O)H structure, the most energetically favored initial reaction is formation of R. + HCOCH=CHCO., but assuming that mechanism results in a model that consistently underpredicts PAN yields in alkylbenzene - NOx chamber experiments. Therefore, a set of products is assumed to be formed that may result from various different reactions, and give predictions of PAN yields that are more consistent with available chamber data.

Footnotes for Table 2.

No.	Note
131	Isoprene mechanism used is based on the "four product" condensed isoprene mechanism of Carter (1996) which in turn is based on the detailed isoprene mechanism of Carter and Atkinson (1996). The rate constants and the major initial reaction pathways are the same as used in those mechanisms. Some minor changes in product yields resulted in some cases from use of the general mechanism estimation system (Carter, 1999a) to generate the overall reaction schemes, or as indicated in other footnotes.
132	The overall nitrate yield is slightly higher than the adjusted nitrate yields in the Carter and Atkinson (1996) mechanism because the mechanism generation system included some nitrate formation from peroxy radicals formed in secondary reactions. Although the yields were not readjusted, the mechanism still gives satisfactory fits to the isoprene chamber data used in the nitrate yield adjustments by Carter and Atkinson (1996).
133	The excited CH_2=CHC(O_2)CH_3 and CH_2=C(CH_3)CHO_2. biradical reactions are the same as given by Carter and Atkinson (1996), except that the CH_2=CHC(O)O_2. formed from the former is represented by MA-RCO3, and the propene formed from the latter is represented by PROD2.
134	All the organic products formed in this reaction are represented by ISOPROD. A small amount of nitrate formation is estimated to occur from the reactions of the substituted peroxy radicals with NO (Carter, 1999a).
135	PROD2 is used to represent the various isoprene oxide products. And MA-RCO3 us used to represent CH_2=CHC(O)OO. Note that this mechanism, which is based on that of Carter and Atkinson (1996) is inconsistent with the mechanisms for the reactions of O^3P with the other higher alkenes, which are assumed not to form radical products. However, assuming no radical formation in the reaction of O^3P with isoprene results in somewhat degraded model performance in simulations of the results of the isoprene experiments discussed by Carter and Atkinson (1996).

Table 3. Listing of the absorption cross sections and quantum yields for the photolysis reactions.

WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY
							NO2							
205.0	4.31e-19	1.000	210.0	4.72e-19	1.000	215.0	4.95e-19	1.000	220.0	4.56e-19	1.000	225.0	3.79e-19	1.000
230.0	2.74e-19	1.000	235.0	1.67e-19	1.000	240.0	9.31e-20	1.000	245.0	4.74e-20	1.000	250.0	2.48e-20	1.000
255.0	1.95e-20	1.000	260.0	2.24e-20	1.000	265.0	2.73e-20	1.000	270.0	4.11e-20	1.000	275.0	4.90e-20	1.000
280.0	5.92e-20	1.000	285.0	7.39e-20	1.000	290.0	9.00e-20	1.000	295.0	1.09e-19	1.000	300.0	1.31e-19	1.000
305.0	1.57e-19	1.000	310.0	1.86e-19	1.000	315.0	2.15e-19	0.990	320.0	2.48e-19	0.990	325.0	2.81e-19	0.990
330.0	3.13e-19	0.990	335.0	3.43e-19	0.990	340.0	3.80e-19	0.990	345.0	4.07e-19	0.990	350.0	4.31e-19	0.990
355.0	4.72e-19	0.990	360.0	4.83e-19	0.980	365.0	5.17e-19	0.980	370.0	5.32e-19	0.980	375.0	5.51e-19	0.980
380.0	5.64e-19	0.970	385.0	5.76e-19	0.970	390.0	5.93e-19	0.960	395.0	5.85e-19	0.935	400.0	6.02e-19	0.820
405.0	5.78e-19	0.355	410.0	6.00e-19	0.130	411.0	5.93e-19	0.110	412.0	5.86e-19	0.094	413.0	5.79e-19	0.083
414.0	5.72e-19	0.070	415.0	5.65e-19	0.059	416.0	5.68e-19	0.048	417.0	5.71e-19	0.039	418.0	5.75e-19	0.030
419.0	5.78e-19	0.023	420.0	5.81e-19	0.018	421.0	5.72e-19	0.012	422.0	5.64e-19	0.008	423.0	5.55e-19	0.004
424.0	5.47e-19	0.000												
							NO3NO							
585.0	2.89e-18	0.000	586.0	3.32e-18	0.050	587.0	4.16e-18	0.100	588.0	5.04e-18	0.150	589.0	6.13e-18	0.200
590.0	5.96e-18	0.250	591.0	5.44e-18	0.280	592.0	5.11e-18	0.310	593.0	4.58e-18	0.340	594.0	4.19e-18	0.370
595.0	4.29e-18	0.400	596.0	4.62e-18	0.370	597.0	4.36e-18	0.340	598.0	3.67e-18	0.310	599.0	3.10e-18	0.280
600.0	2.76e-18	0.250	601.0	2.86e-18	0.240	602.0	3.32e-18	0.230	603.0	3.80e-18	0.220	604.0	4.37e-18	0.210
605.0	4.36e-18	0.200	606.0	3.32e-18	0.200	607.0	2.40e-18	0.200	608.0	1.85e-18	0.200	609.0	1.71e-18	0.200
610.0	1.77e-18	0.200	611.0	1.91e-18	0.180	612.0	2.23e-18	0.160	613.0	2.63e-18	0.140	614.0	2.55e-18	0.120
615.0	2.26e-18	0.100	616.0	2.09e-18	0.100	617.0	2.11e-18	0.100	618.0	2.39e-18	0.100	619.0	2.56e-18	0.100
620.0	3.27e-18	0.100	621.0	5.24e-18	0.090	622.0	1.02e-17	0.080	623.0	1.47e-17	0.070	624.0	1.21e-17	0.060
625.0	8.38e-18	0.050	626.0	7.30e-18	0.050	627.0	7.53e-18	0.050	628.0	7.37e-18	0.050	629.0	6.98e-18	0.050
630.0	6.76e-18	0.050	631.0	4.84e-18	0.046	632.0	3.27e-18	0.042	633.0	2.17e-18	0.038	634.0	1.64e-18	0.034
635.0	1.44e-18	0.030	636.0	1.69e-18	0.024	637.0	2.07e-18	0.018	638.0	2.03e-18	0.012	639.0	1.58e-18	0.006
640.0	1.23e-18	0.000												
							NO3NO2							
400.0	0.00e+00	1.000	401.0	0.00e+00	1.000	402.0	0.00e+00	1.000	403.0	2.00e-20	1.000	404.0	0.00e+00	1.000
405.0	3.00e-20	1.000	406.0	2.00e-20	1.000	407.0	1.00e-20	1.000	408.0	3.00e-20	1.000	409.0	0.00e+00	1.000
410.0	1.00e-20	1.000	411.0	2.00e-20	1.000	412.0	5.00e-20	1.000	413.0	5.00e-20	1.000	414.0	2.00e-20	1.000
415.0	6.00e-20	1.000	416.0	6.00e-20	1.000	417.0	7.00e-20	1.000	418.0	5.00e-20	1.000	419.0	8.00e-20	1.000
420.0	8.00e-20	1.000	421.0	8.00e-20	1.000	422.0	9.00e-20	1.000	423.0	1.10e-19	1.000	424.0	9.00e-20	1.000
425.0	7.00e-20	1.000	426.0	1.40e-19	1.000	427.0	1.40e-19	1.000	428.0	1.20e-19	1.000	429.0	1.10e-19	1.000
430.0	1.70e-19	1.000	431.0	1.30e-19	1.000	432.0	1.50e-19	1.000	433.0	1.80e-19	1.000	434.0	1.80e-19	1.000
435.0	1.60e-19	1.000	436.0	1.50e-19	1.000	437.0	1.80e-19	1.000	438.0	2.10e-19	1.000	439.0	2.00e-19	1.000
440.0	1.90e-19	1.000	441.0	1.80e-19	1.000	442.0	2.10e-19	1.000	443.0	1.80e-19	1.000	444.0	1.90e-19	1.000
445.0	2.00e-19	1.000	446.0	2.40e-19	1.000	447.0	2.90e-19	1.000	448.0	2.40e-19	1.000	449.0	2.80e-19	1.000
450.0	2.90e-19	1.000	451.0	3.00e-19	1.000	452.0	3.30e-19	1.000	453.0	3.10e-19	1.000	454.0	3.60e-19	1.000
455.0	3.60e-19	1.000	456.0	3.60e-19	1.000	457.0	4.00e-19	1.000	458.0	3.70e-19	1.000	459.0	4.20e-19	1.000
460.0	4.00e-19	1.000	461.0	3.90e-19	1.000	462.0	4.00e-19	1.000	463.0	4.10e-19	1.000	464.0	4.80e-19	1.000
465.0	5.10e-19	1.000	466.0	5.40e-19	1.000	467.0	5.70e-19	1.000	468.0	5.60e-19	1.000	469.0	5.80e-19	1.000
470.0	5.90e-19	1.000	471.0	6.20e-19	1.000	472.0	6.40e-19	1.000	473.0	6.20e-19	1.000	474.0	6.20e-19	1.000
475.0	6.80e-19	1.000	476.0	7.80e-19	1.000	477.0	7.70e-19	1.000	478.0	7.30e-19	1.000	479.0	7.30e-19	1.000
480.0	7.00e-19	1.000	481.0	7.10e-19	1.000	482.0	7.10e-19	1.000	483.0	7.20e-19	1.000	484.0	7.70e-19	1.000
485.0	8.20e-19	1.000	486.0	9.10e-19	1.000	487.0	9.20e-19	1.000	488.0	9.50e-19	1.000	489.0	9.60e-19	1.000
490.0	1.03e-18	1.000	491.0	9.90e-19	1.000	492.0	9.90e-19	1.000	493.0	1.01e-18	1.000	494.0	1.01e-18	1.000
495.0	1.06e-18	1.000	496.0	1.21e-18	1.000	497.0	1.22e-18	1.000	498.0	1.20e-18	1.000	499.0	1.17e-18	1.000
500.0	1.13e-18	1.000	501.0	1.11e-18	1.000	502.0	1.11e-18	1.000	503.0	1.11e-18	1.000	504.0	1.26e-18	1.000
505.0	1.28e-18	1.000	506.0	1.34e-18	1.000	507.0	1.28e-18	1.000	508.0	1.27e-18	1.000	509.0	1.35e-18	1.000
510.0	1.51e-18	1.000	511.0	1.73e-18	1.000	512.0	1.77e-18	1.000	513.0	1.60e-18	1.000	514.0	1.58e-18	1.000
515.0	1.58e-18	1.000	516.0	1.56e-18	1.000	517.0	1.49e-18	1.000	518.0	1.44e-18	1.000	519.0	1.54e-18	1.000

WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY
520.0	1.68e-18	1.000	521.0	1.83e-18	1.000	522.0	1.93e-18	1.000	523.0	1.77e-18	1.000	524.0	1.64e-18	1.000
525.0	1.58e-18	1.000	526.0	1.63e-18	1.000	527.0	1.81e-18	1.000	528.0	2.10e-18	1.000	529.0	2.39e-18	1.000
530.0	2.23e-18	1.000	531.0	2.09e-18	1.000	532.0	2.02e-18	1.000	533.0	1.95e-18	1.000	534.0	2.04e-18	1.000
535.0	2.30e-18	1.000	536.0	2.57e-18	1.000	537.0	2.58e-18	1.000	538.0	2.34e-18	1.000	539.0	2.04e-18	1.000
540.0	2.10e-18	1.000	541.0	2.04e-18	1.000	542.0	1.88e-18	1.000	543.0	1.68e-18	1.000	544.0	1.70e-18	1.000
545.0	1.96e-18	1.000	546.0	2.42e-18	1.000	547.0	2.91e-18	1.000	548.0	2.98e-18	1.000	549.0	2.71e-18	1.000
550.0	2.48e-18	1.000	551.0	2.43e-18	1.000	552.0	2.47e-18	1.000	553.0	2.53e-18	1.000	554.0	2.78e-18	1.000
555.0	3.11e-18	1.000	556.0	3.26e-18	1.000	557.0	3.29e-18	1.000	558.0	3.51e-18	1.000	559.0	3.72e-18	1.000
560.0	3.32e-18	1.000	561.0	2.98e-18	1.000	562.0	2.90e-18	1.000	563.0	2.80e-18	1.000	564.0	2.72e-18	1.000
565.0	2.73e-18	1.000	566.0	2.85e-18	1.000	567.0	2.81e-18	1.000	568.0	2.85e-18	1.000	569.0	2.89e-18	1.000
570.0	2.79e-18	1.000	571.0	2.76e-18	1.000	572.0	2.74e-18	1.000	573.0	2.78e-18	1.000	574.0	2.86e-18	1.000
575.0	3.08e-18	1.000	576.0	3.27e-18	1.000	577.0	3.38e-18	1.000	578.0	3.31e-18	1.000	579.0	3.24e-18	1.000
580.0	3.34e-18	1.000	581.0	3.55e-18	1.000	582.0	3.28e-18	1.000	583.0	2.93e-18	1.000	584.0	2.82e-18	1.000
585.0	2.89e-18	1.000	586.0	3.32e-18	0.950	587.0	4.16e-18	0.900	588.0	5.04e-18	0.850	589.0	6.13e-18	0.800
590.0	5.96e-18	0.750	591.0	5.44e-18	0.720	592.0	5.11e-18	0.690	593.0	4.58e-18	0.660	594.0	4.19e-18	0.630
595.0	4.29e-18	0.600	596.0	4.62e-18	0.590	597.0	4.36e-18	0.580	598.0	3.67e-18	0.570	599.0	3.10e-18	0.560
600.0	2.76e-18	0.550	601.0	2.86e-18	0.540	602.0	3.32e-18	0.530	603.0	3.80e-18	0.520	604.0	4.37e-18	0.510
605.0	4.36e-18	0.400	606.0	3.32e-18	0.380	607.0	2.40e-18	0.360	608.0	1.85e-18	0.340	609.0	1.71e-18	0.320
610.0	1.77e-18	0.300	611.0	1.91e-18	0.290	612.0	2.23e-18	0.280	613.0	2.63e-18	0.270	614.0	2.55e-18	0.260
615.0	2.26e-18	0.250	616.0	2.09e-18	0.240	617.0	2.11e-18	0.230	618.0	2.39e-18	0.220	619.0	2.56e-18	0.210
620.0	3.27e-18	0.200	621.0	5.24e-18	0.190	622.0	1.02e-17	0.180	623.0	1.47e-17	0.170	624.0	1.21e-17	0.160
625.0	8.38e-18	0.150	626.0	7.30e-18	0.130	627.0	7.53e-18	0.110	628.0	7.37e-18	0.090	629.0	6.98e-18	0.070
630.0	6.76e-18	0.050	631.0	4.84e-18	0.040	632.0	3.27e-18	0.030	633.0	2.17e-18	0.020	634.0	1.64e-18	0.010
635.0	1.44e-18	0.000												

O3O3P

175.4	8.11e-19	0.050	177.0	8.11e-19	0.050	178.6	7.99e-19	0.050	180.2	7.86e-19	0.050	181.8	7.63e-19	0.050
183.5	7.29e-19	0.050	185.2	6.88e-19	0.050	186.9	6.22e-19	0.050	188.7	5.76e-19	0.050	190.5	5.26e-19	0.050
192.3	4.76e-19	0.050	194.2	4.28e-19	0.050	196.1	3.83e-19	0.050	198.0	3.47e-19	0.050	200.0	3.23e-19	0.050
202.0	3.14e-19	0.050	204.1	3.26e-19	0.050	206.2	3.64e-19	0.050	208.3	4.34e-19	0.050	210.5	5.42e-19	0.050
212.8	6.99e-19	0.050	215.0	9.20e-19	0.050	217.4	1.19e-18	0.050	219.8	1.55e-18	0.050	222.2	1.99e-18	0.050
224.7	2.56e-18	0.050	227.3	3.23e-18	0.050	229.9	4.00e-18	0.050	232.6	4.83e-18	0.050	235.3	5.79e-18	0.050
238.1	6.86e-18	0.050	241.0	7.97e-18	0.050	243.9	9.00e-18	0.050	246.9	1.00e-17	0.050	250.1	1.08e-17	0.050
253.2	1.13e-17	0.050	256.4	1.15e-17	0.050	259.7	1.12e-17	0.050	263.2	1.06e-17	0.050	266.7	9.65e-18	0.050
270.3	8.34e-18	0.050	274.0	6.92e-18	0.050	277.8	5.42e-18	0.050	281.7	4.02e-18	0.050	285.7	2.77e-18	0.050
289.9	1.79e-18	0.050	290.0	1.77e-18	0.050	294.1	1.09e-18	0.050	295.0	9.95e-19	0.050	298.5	6.24e-19	0.050
300.0	5.30e-19	0.050	303.0	3.43e-19	0.015	305.0	2.76e-19	0.020	306.0	2.42e-19	0.050	307.0	2.09e-19	0.123
307.7	1.85e-19	0.196	308.0	1.80e-19	0.227	309.0	1.61e-19	0.333	310.0	1.43e-19	0.400	311.0	1.25e-19	0.612
312.0	1.07e-19	0.697	312.5	9.80e-20	0.718	313.0	9.32e-20	0.738	314.0	8.36e-20	0.762	315.0	7.40e-20	0.765
316.0	6.44e-20	0.779	317.0	5.48e-20	0.791	317.5	5.00e-20	0.799	318.0	4.75e-20	0.806	319.0	4.25e-20	0.822
322.5	2.49e-20	0.906	327.5	1.20e-20	0.940	332.5	6.17e-21	0.950	337.5	2.74e-21	0.975	342.5	1.17e-21	1.000
347.5	5.90e-22	1.000	352.5	2.70e-22	1.000	357.5	1.10e-22	1.000	362.5	5.00e-23	1.000	367.5	0.00e+00	1.000
400.0	0.00e+00	1.000	410.0	1.20e-23	1.000	420.0	2.20e-23	1.000	440.0	1.12e-22	1.000	460.0	3.28e-22	1.000
480.0	6.84e-22	1.000	500.0	1.22e-21	1.000	520.0	1.82e-21	1.000	540.0	2.91e-21	1.000	560.0	3.94e-21	1.000
580.0	4.59e-21	1.000	600.0	5.11e-21	1.000	620.0	4.00e-21	1.000	640.0	2.96e-21	1.000	660.0	2.09e-21	1.000
680.0	1.36e-21	1.000	700.0	9.10e-22	1.000	750.0	3.20e-22	1.000	800.0	1.60e-22	1.000	900.0	0.00e+00	1.000

O3O1D

175.4	8.11e-19	0.870	177.0	8.11e-19	0.870	178.6	7.99e-19	0.870	180.2	7.86e-19	0.870	181.8	7.63e-19	0.870
183.5	7.29e-19	0.870	185.2	6.88e-19	0.870	186.9	6.22e-19	0.870	188.7	5.76e-19	0.870	190.5	5.26e-19	0.870
192.3	4.76e-19	0.870	194.2	4.28e-19	0.870	196.1	3.83e-19	0.870	198.0	3.47e-19	0.870	200.0	3.23e-19	0.870
202.0	3.14e-19	0.870	204.1	3.26e-19	0.870	206.2	3.64e-19	0.870	208.3	4.34e-19	0.870	210.5	5.42e-19	0.870
212.8	6.99e-19	0.870	215.0	9.20e-19	0.870	217.4	1.19e-18	0.870	219.8	1.55e-18	0.870	222.2	1.99e-18	0.870
224.7	2.56e-18	0.870	227.3	3.23e-18	0.870	229.9	4.00e-18	0.870	232.6	4.83e-18	0.870	235.3	5.79e-18	0.870
238.1	6.86e-18	0.870	241.0	7.97e-18	0.870	243.9	9.00e-18	0.870	246.9	1.00e-17	0.870	250.1	1.08e-17	0.870

WL (nm)	Abs (cm^2)	QY (nm)	WL	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY
253.2	1.13e-17	0.870	256.4	1.15e-17	0.870	259.7	1.12e-17	0.870	263.2	1.06e-17	0.870	266.7	9.65e-18	0.870
270.3	8.34e-18	0.870	274.0	6.92e-18	0.881	277.8	5.42e-18	0.896	281.7	4.02e-18	0.911	285.7	2.77e-18	0.926
289.9	1.79e-18	0.942	290.0	1.77e-18	0.942	294.1	1.09e-18	0.950	295.0	9.95e-19	0.950	298.5	6.24e-19	0.950
300.0	5.30e-19	0.950	303.0	3.43e-19	0.985	305.0	2.76e-19	0.980	306.0	2.42e-19	0.950	307.0	2.09e-19	0.877
307.7	1.85e-19	0.804	308.0	1.80e-19	0.773	309.0	1.61e-19	0.667	310.0	1.43e-19	0.600	311.0	1.25e-19	0.388
312.0	1.07e-19	0.303	312.5	9.80e-20	0.283	313.0	9.32e-20	0.262	314.0	8.36e-20	0.238	315.0	7.40e-20	0.235
316.0	6.44e-20	0.221	317.0	5.48e-20	0.209	317.5	5.00e-20	0.202	318.0	4.75e-20	0.194	319.0	4.25e-20	0.178
322.5	2.49e-20	0.095	327.5	1.20e-20	0.060	332.5	6.17e-21	0.050	337.5	2.74e-21	0.025	342.5	1.17e-21	0.000
347.5	5.90e-22	0.000												

HONO-NO

311.0	0.00e+00	0.411	312.0	2.00e-21	0.421	313.0	4.20e-21	0.432	314.0	4.60e-21	0.443	315.0	4.20e-21	0.454
316.0	3.00e-21	0.464	317.0	4.60e-21	0.475	318.0	3.60e-20	0.486	319.0	6.10e-20	0.496	320.0	2.10e-20	0.507
321.0	4.27e-20	0.518	322.0	4.01e-20	0.529	323.0	3.93e-20	0.539	324.0	4.01e-20	0.550	325.0	4.04e-20	0.561
326.0	3.13e-20	0.571	327.0	4.12e-20	0.582	328.0	7.55e-20	0.593	329.0	6.64e-20	0.604	330.0	7.29e-20	0.614
331.0	8.70e-20	0.625	332.0	1.38e-19	0.636	333.0	5.91e-20	0.646	334.0	5.91e-20	0.657	335.0	6.45e-20	0.668
336.0	5.91e-20	0.679	337.0	4.58e-20	0.689	338.0	1.91e-19	0.700	339.0	1.63e-19	0.711	340.0	1.05e-19	0.721
341.0	8.70e-20	0.732	342.0	3.35e-19	0.743	343.0	2.01e-19	0.754	344.0	1.02e-19	0.764	345.0	8.54e-20	0.775
346.0	8.32e-20	0.786	347.0	8.20e-20	0.796	348.0	7.49e-20	0.807	349.0	7.13e-20	0.818	350.0	6.83e-20	0.829
351.0	1.74e-19	0.839	352.0	1.14e-19	0.850	353.0	3.71e-19	0.861	354.0	4.96e-19	0.871	355.0	2.46e-19	0.882
356.0	1.19e-19	0.893	357.0	9.35e-20	0.904	358.0	7.78e-20	0.914	359.0	7.29e-20	0.925	360.0	6.83e-20	0.936
361.0	6.90e-20	0.946	362.0	7.32e-20	0.957	363.0	9.00e-20	0.968	364.0	1.21e-19	0.979	365.0	1.33e-19	0.989
366.0	2.13e-19	1.000	367.0	3.52e-19	1.000	368.0	4.50e-19	1.000	369.0	2.93e-19	1.000	370.0	1.19e-19	1.000
371.0	9.46e-20	1.000	372.0	8.85e-20	1.000	373.0	7.44e-20	1.000	374.0	4.77e-20	1.000	375.0	2.70e-20	1.000
376.0	1.90e-20	1.000	377.0	1.50e-20	1.000	378.0	1.90e-20	1.000	379.0	5.80e-20	1.000	380.0	7.78e-20	1.000
381.0	1.14e-19	1.000	382.0	1.40e-19	1.000	383.0	1.72e-19	1.000	384.0	1.99e-19	1.000	385.0	1.90e-19	1.000
386.0	1.19e-19	1.000	387.0	5.65e-20	1.000	388.0	3.20e-20	1.000	389.0	1.90e-20	1.000	390.0	1.20e-20	1.000
391.0	5.00e-21	1.000	392.0	0.00e+00	1.000									

HONO-NO2

311.0	0.00e+00	0.589	312.0	2.00e-21	0.579	313.0	4.20e-21	0.568	314.0	4.60e-21	0.557	315.0	4.20e-21	0.546
316.0	3.00e-21	0.536	317.0	4.60e-21	0.525	318.0	3.60e-20	0.514	319.0	6.10e-20	0.504	320.0	2.10e-20	0.493
321.0	4.27e-20	0.482	322.0	4.01e-20	0.471	323.0	3.93e-20	0.461	324.0	4.01e-20	0.450	325.0	4.04e-20	0.439
326.0	3.13e-20	0.429	327.0	4.12e-20	0.418	328.0	7.55e-20	0.407	329.0	6.64e-20	0.396	330.0	7.29e-20	0.386
331.0	8.70e-20	0.375	332.0	1.38e-19	0.364	333.0	5.91e-20	0.354	334.0	5.91e-20	0.343	335.0	6.45e-20	0.332
336.0	5.91e-20	0.321	337.0	4.58e-20	0.311	338.0	1.91e-19	0.300	339.0	1.63e-19	0.289	340.0	1.05e-19	0.279
341.0	8.70e-20	0.268	342.0	3.35e-19	0.257	343.0	2.01e-19	0.246	344.0	1.02e-19	0.236	345.0	8.54e-20	0.225
346.0	8.32e-20	0.214	347.0	8.20e-20	0.204	348.0	7.49e-20	0.193	349.0	7.13e-20	0.182	350.0	6.83e-20	0.171
351.0	1.74e-19	0.161	352.0	1.14e-19	0.150	353.0	3.71e-19	0.139	354.0	4.96e-19	0.129	355.0	2.46e-19	0.118
356.0	1.19e-19	0.107	357.0	9.35e-20	0.096	358.0	7.78e-20	0.086	359.0	7.29e-20	0.075	360.0	6.83e-20	0.064
361.0	6.90e-20	0.054	362.0	7.32e-20	0.043	363.0	9.00e-20	0.032	364.0	1.21e-19	0.021	365.0	1.33e-19	0.011
366.0	2.13e-19	0.000												

HNO3

190.0	1.36e-17	1.000	195.0	1.02e-17	1.000	200.0	5.88e-18	1.000	205.0	2.80e-18	1.000	210.0	1.04e-18	1.000
215.0	3.65e-19	1.000	220.0	1.49e-19	1.000	225.0	8.81e-20	1.000	230.0	5.75e-20	1.000	235.0	3.75e-20	1.000
240.0	2.58e-20	1.000	245.0	2.11e-20	1.000	250.0	1.97e-20	1.000	255.0	1.95e-20	1.000	260.0	1.91e-20	1.000
265.0	1.80e-20	1.000	270.0	1.62e-20	1.000	275.0	1.38e-20	1.000	280.0	1.12e-20	1.000	285.0	8.58e-21	1.000
290.0	6.15e-21	1.000	295.0	4.12e-21	1.000	300.0	2.63e-21	1.000	305.0	1.50e-21	1.000	310.0	8.10e-22	1.000
315.0	4.10e-22	1.000	320.0	2.00e-22	1.000	325.0	9.50e-23	1.000	330.0	4.30e-23	1.000	335.0	2.20e-23	1.000
340.0	1.00e-23	1.000	345.0	6.00e-24	1.000	350.0	4.00e-24	1.000	355.0	0.00e+00	1.000			

HO2NO2

190.0	1.01e-17	1.000	195.0	8.16e-18	1.000	200.0	5.63e-18	1.000	205.0	3.67e-18	1.000	210.0	2.39e-18	1.000
215.0	1.61e-18	1.000	220.0	1.18e-18	1.000	225.0	9.32e-19	1.000	230.0	7.88e-19	1.000	235.0	6.80e-19	1.000
240.0	5.79e-19	1.000	245.0	4.97e-19	1.000	250.0	4.11e-19	1.000	255.0	3.49e-19	1.000	260.0	2.84e-19	1.000

WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY
265.0	2.29e-19	1.000	270.0	1.80e-19	1.000	275.0	1.33e-19	1.000	280.0	9.30e-20	1.000	285.0	6.20e-20	1.000
290.0	3.90e-20	1.000	295.0	2.40e-20	1.000	300.0	1.40e-20	1.000	305.0	8.50e-21	1.000	310.0	5.30e-21	1.000
315.0	3.90e-21	1.000	320.0	2.40e-21	1.000	325.0	1.50e-21	1.000	330.0	9.00e-22	1.000	335.0	0.00e+00	1.000
H2O2														
190.0	6.72e-19	1.000	195.0	5.63e-19	1.000	200.0	4.75e-19	1.000	205.0	4.08e-19	1.000	210.0	3.57e-19	1.000
215.0	3.07e-19	1.000	220.0	2.58e-19	1.000	225.0	2.17e-19	1.000	230.0	1.82e-19	1.000	235.0	1.50e-19	1.000
240.0	1.24e-19	1.000	245.0	1.02e-19	1.000	250.0	8.30e-20	1.000	255.0	6.70e-20	1.000	260.0	5.30e-20	1.000
265.0	4.20e-20	1.000	270.0	3.30e-20	1.000	275.0	2.60e-20	1.000	280.0	2.00e-20	1.000	285.0	1.50e-20	1.000
290.0	1.20e-20	1.000	295.0	9.00e-21	1.000	300.0	6.80e-21	1.000	305.0	5.10e-21	1.000	310.0	3.90e-21	1.000
315.0	2.90e-21	1.000	320.0	2.20e-21	1.000	325.0	1.60e-21	1.000	330.0	1.30e-21	1.000	335.0	1.00e-21	1.000
340.0	7.00e-22	1.000	345.0	5.00e-22	1.000	350.0	4.00e-22	1.000	355.0	0.00e+00	1.000			
HCHO_R														
240.0	6.40e-22	0.270	241.0	5.60e-22	0.272	242.0	1.05e-21	0.274	243.0	1.15e-21	0.276	244.0	8.20e-22	0.278
245.0	1.03e-21	0.280	246.0	9.80e-22	0.282	247.0	1.35e-21	0.284	248.0	1.91e-21	0.286	249.0	2.82e-21	0.288
250.0	2.05e-21	0.290	251.0	1.70e-21	0.291	252.0	2.88e-21	0.292	253.0	2.55e-21	0.293	254.0	2.55e-21	0.294
255.0	3.60e-21	0.295	256.0	5.09e-21	0.296	257.0	3.39e-21	0.297	258.0	2.26e-21	0.298	259.0	5.04e-21	0.299
260.0	5.05e-21	0.300	261.0	5.49e-21	0.308	262.0	5.20e-21	0.316	263.0	9.33e-21	0.324	264.0	8.23e-21	0.332
265.0	4.30e-21	0.340	266.0	4.95e-21	0.348	267.0	1.24e-20	0.356	268.0	1.11e-20	0.364	269.0	8.78e-21	0.372
270.0	9.36e-21	0.380	271.0	1.79e-20	0.399	272.0	1.23e-20	0.418	273.0	6.45e-21	0.437	274.0	6.56e-21	0.456
275.0	2.23e-20	0.475	276.0	2.42e-20	0.494	277.0	1.40e-20	0.513	278.0	1.05e-20	0.532	279.0	2.55e-20	0.551
280.0	2.08e-20	0.570	281.0	1.48e-20	0.586	282.0	8.81e-21	0.602	283.0	1.07e-20	0.618	284.0	4.49e-20	0.634
285.0	3.59e-20	0.650	286.0	1.96e-20	0.666	287.0	1.30e-20	0.682	288.0	3.36e-20	0.698	289.0	2.84e-20	0.714
290.0	1.30e-20	0.730	291.0	1.75e-20	0.735	292.0	8.32e-21	0.740	293.0	3.73e-20	0.745	294.0	6.54e-20	0.750
295.0	3.95e-20	0.755	296.0	2.33e-20	0.760	297.0	1.51e-20	0.765	298.0	4.04e-20	0.770	299.0	2.87e-20	0.775
300.0	8.71e-21	0.780	301.0	1.72e-20	0.780	302.0	1.06e-20	0.780	303.0	3.20e-20	0.780	304.0	6.90e-20	0.780
305.0	4.91e-20	0.780	306.0	4.63e-20	0.780	307.0	2.10e-20	0.780	308.0	1.49e-20	0.780	309.0	3.41e-20	0.780
310.0	1.95e-20	0.780	311.0	5.21e-21	0.764	312.0	1.12e-20	0.748	313.0	1.12e-20	0.732	314.0	4.75e-20	0.716
315.0	5.25e-20	0.700	316.0	2.90e-20	0.684	317.0	5.37e-20	0.668	318.0	2.98e-20	0.652	319.0	9.18e-21	0.636
320.0	1.26e-20	0.620	321.0	1.53e-20	0.585	322.0	6.69e-21	0.550	323.0	3.45e-21	0.515	324.0	8.16e-21	0.480
325.0	1.85e-20	0.445	326.0	5.95e-20	0.410	327.0	3.49e-20	0.375	328.0	1.09e-20	0.340	329.0	3.35e-20	0.305
330.0	3.32e-20	0.270	331.0	1.07e-20	0.243	332.0	2.89e-21	0.216	333.0	2.15e-21	0.189	334.0	1.71e-21	0.162
335.0	1.43e-21	0.135	336.0	1.94e-21	0.108	337.0	4.17e-21	0.081	338.0	2.36e-20	0.054	339.0	4.71e-20	0.027
340.0	2.48e-20	0.000												
HCHO_M														
240.0	6.40e-22	0.490	241.0	5.60e-22	0.490	242.0	1.05e-21	0.490	243.0	1.15e-21	0.490	244.0	8.20e-22	0.490
245.0	1.03e-21	0.490	246.0	9.80e-22	0.490	247.0	1.35e-21	0.490	248.0	1.91e-21	0.490	249.0	2.82e-21	0.490
250.0	2.05e-21	0.490	251.0	1.70e-21	0.490	252.0	2.88e-21	0.490	253.0	2.55e-21	0.490	254.0	2.55e-21	0.490
255.0	3.60e-21	0.490	256.0	5.09e-21	0.490	257.0	3.39e-21	0.490	258.0	2.26e-21	0.490	259.0	5.04e-21	0.490
260.0	5.05e-21	0.490	261.0	5.49e-21	0.484	262.0	5.20e-21	0.478	263.0	9.33e-21	0.472	264.0	8.23e-21	0.466
265.0	4.30e-21	0.460	266.0	4.95e-21	0.454	267.0	1.24e-20	0.448	268.0	1.11e-20	0.442	269.0	8.78e-21	0.436
270.0	9.36e-21	0.430	271.0	1.79e-20	0.419	272.0	1.23e-20	0.408	273.0	6.45e-21	0.397	274.0	6.56e-21	0.386
275.0	2.23e-20	0.375	276.0	2.42e-20	0.364	277.0	1.40e-20	0.353	278.0	1.05e-20	0.342	279.0	2.55e-20	0.331
280.0	2.08e-20	0.320	281.0	1.48e-20	0.312	282.0	8.81e-21	0.304	283.0	1.07e-20	0.296	284.0	4.49e-20	0.288
285.0	3.59e-20	0.280	286.0	1.96e-20	0.272	287.0	1.30e-20	0.264	288.0	3.36e-20	0.256	289.0	2.84e-20	0.248
290.0	1.30e-20	0.240	291.0	1.75e-20	0.237	292.0	8.32e-21	0.234	293.0	3.73e-20	0.231	294.0	6.54e-20	0.228
295.0	3.95e-20	0.225	296.0	2.33e-20	0.222	297.0	1.51e-20	0.219	298.0	4.04e-20	0.216	299.0	2.87e-20	0.213
300.0	8.71e-21	0.210	301.0	1.72e-20	0.211	302.0	1.06e-20	0.212	303.0	3.20e-20	0.213	304.0	6.90e-20	0.214
305.0	4.91e-20	0.215	306.0	4.63e-20	0.216	307.0	2.10e-20	0.217	308.0	1.49e-20	0.218	309.0	3.41e-20	0.219
310.0	1.95e-20	0.220	311.0	5.21e-21	0.236	312.0	1.12e-20	0.252	313.0	1.12e-20	0.268	314.0	4.75e-20	0.284
315.0	5.25e-20	0.300	316.0	2.90e-20	0.316	317.0	5.37e-20	0.332	318.0	2.98e-20	0.348	319.0	9.18e-21	0.364
320.0	1.26e-20	0.380	321.0	1.53e-20	0.408	322.0	6.69e-21	0.436	323.0	3.45e-21	0.464	324.0	8.16e-21	0.492
325.0	1.85e-20	0.520	326.0	5.95e-20	0.548	327.0	3.49e-20	0.576	328.0	1.09e-20	0.604	329.0	3.35e-20	0.632

WL (nm)	Abs (cm^2)	QY (nm)	WL	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY
330.0	3.32e-20	0.660	331.0	1.07e-20	0.650	332.0	2.89e-21	0.640	333.0	2.15e-21	0.630	334.0	1.71e-21	0.620
335.0	1.43e-21	0.610	336.0	1.94e-21	0.600	337.0	4.17e-21	0.590	338.0	2.36e-20	0.580	339.0	4.71e-20	0.570
340.0	2.48e-20	0.560	341.0	7.59e-21	0.525	342.0	6.81e-21	0.490	343.0	1.95e-20	0.455	344.0	1.14e-20	0.420
345.0	3.23e-21	0.385	346.0	1.13e-21	0.350	347.0	6.60e-22	0.315	348.0	1.22e-21	0.280	349.0	3.20e-22	0.245
350.0	3.80e-22	0.210	351.0	1.04e-21	0.192	352.0	7.13e-21	0.174	353.0	2.21e-20	0.156	354.0	1.54e-20	0.138
355.0	6.76e-21	0.120	356.0	1.35e-21	0.102	357.0	3.60e-22	0.084	358.0	5.70e-23	0.066	359.0	5.80e-22	0.048
360.0	8.20e-22	0.000												
						CCHO_R								
262.0	2.44e-20	0.326	266.0	3.05e-20	0.358	270.0	3.42e-20	0.390	274.0	4.03e-20	0.466	278.0	4.19e-20	0.542
280.0	4.50e-20	0.580	281.0	4.69e-20	0.575	282.0	4.72e-20	0.570	283.0	4.75e-20	0.565	284.0	4.61e-20	0.560
285.0	4.49e-20	0.555	286.0	4.44e-20	0.550	287.0	4.59e-20	0.545	288.0	4.72e-20	0.540	289.0	4.77e-20	0.535
290.0	4.89e-20	0.530	291.0	4.78e-20	0.520	292.0	4.68e-20	0.510	293.0	4.53e-20	0.500	294.0	4.33e-20	0.490
295.0	4.27e-20	0.480	296.0	4.24e-20	0.470	297.0	4.38e-20	0.460	298.0	4.41e-20	0.450	299.0	4.26e-20	0.440
300.0	4.16e-20	0.430	301.0	3.99e-20	0.418	302.0	3.86e-20	0.406	303.0	3.72e-20	0.394	304.0	3.48e-20	0.382
305.0	3.42e-20	0.370	306.0	3.42e-20	0.354	307.0	3.36e-20	0.338	308.0	3.33e-20	0.322	309.0	3.14e-20	0.306
310.0	2.93e-20	0.290	311.0	2.76e-20	0.266	312.0	2.53e-20	0.242	313.0	2.47e-20	0.218	314.0	2.44e-20	0.194
315.0	2.20e-20	0.170	316.0	2.04e-20	0.156	317.0	2.07e-20	0.142	318.0	1.98e-20	0.128	319.0	1.87e-20	0.114
320.0	1.72e-20	0.100	321.0	1.48e-20	0.088	322.0	1.40e-20	0.076	323.0	1.24e-20	0.064	324.0	1.09e-20	0.052
325.0	1.14e-20	0.040	326.0	1.07e-20	0.032	327.0	8.58e-21	0.024	328.0	7.47e-21	0.016	329.0	7.07e-21	0.008
						C2CHO								
294.0	5.80e-20	0.890	295.0	5.57e-20	0.885	296.0	5.37e-20	0.880	297.0	5.16e-20	0.875	298.0	5.02e-20	0.870
299.0	5.02e-20	0.865	300.0	5.04e-20	0.860	301.0	5.09e-20	0.855	302.0	5.07e-20	0.850	303.0	4.94e-20	0.818
304.0	4.69e-20	0.786	305.0	4.32e-20	0.755	306.0	4.04e-20	0.723	307.0	3.81e-20	0.691	308.0	3.65e-20	0.659
309.0	3.62e-20	0.627	310.0	3.60e-20	0.596	311.0	3.53e-20	0.564	312.0	3.50e-20	0.532	313.0	3.32e-20	0.500
314.0	3.06e-20	0.480	315.0	2.77e-20	0.460	316.0	2.43e-20	0.440	317.0	2.18e-20	0.420	318.0	2.00e-20	0.400
319.0	1.86e-20	0.380	320.0	1.83e-20	0.360	321.0	1.78e-20	0.340	322.0	1.66e-20	0.320	323.0	1.58e-20	0.300
324.0	1.49e-20	0.280	325.0	1.30e-20	0.260	326.0	1.13e-20	0.248	327.0	9.96e-21	0.236	328.0	8.28e-21	0.223
329.0	6.85e-21	0.211	330.0	5.75e-21	0.199	331.0	4.94e-21	0.187	332.0	4.66e-21	0.174	333.0	4.30e-21	0.162
334.0	3.73e-21	0.150	335.0	3.25e-21	0.133	336.0	2.80e-21	0.117	337.0	2.30e-21	0.100	338.0	1.85e-21	0.083
339.0	1.66e-21	0.067	340.0	1.55e-21	0.050	341.0	1.19e-21	0.033	342.0	7.60e-22	0.017	343.0	4.50e-22	0.000
						KETONE								
198.5	3.95e-19	1.000	199.0	1.61e-19	1.000	199.5	7.75e-20	1.000	200.0	3.76e-20	1.000	200.5	2.51e-20	1.000
201.0	1.83e-20	1.000	201.5	1.36e-20	1.000	202.0	1.16e-20	1.000	202.5	8.97e-21	1.000	203.0	4.62e-21	1.000
203.5	3.18e-21	1.000	204.0	2.42e-21	1.000	204.5	2.01e-21	1.000	205.0	1.77e-21	1.000	205.5	1.64e-21	1.000
206.0	1.54e-21	1.000	206.5	1.52e-21	1.000	207.0	1.54e-21	1.000	207.5	1.62e-21	1.000	208.0	1.64e-21	1.000
208.5	1.60e-21	1.000	209.0	1.57e-21	1.000	209.5	1.49e-21	1.000	210.0	1.47e-21	1.000	210.5	1.52e-21	1.000
211.0	1.50e-21	1.000	211.5	1.62e-21	1.000	212.0	1.81e-21	1.000	212.5	2.10e-21	1.000	213.0	2.23e-21	1.000
213.5	2.06e-21	1.000	214.0	1.69e-21	1.000	214.5	1.49e-21	1.000	215.0	1.42e-21	1.000	215.5	1.42e-21	1.000
216.0	1.42e-21	1.000	216.5	1.48e-21	1.000	217.0	1.48e-21	1.000	217.5	1.53e-21	1.000	218.0	1.56e-21	1.000
218.5	1.67e-21	1.000	219.0	1.68e-21	1.000	219.5	1.78e-21	1.000	220.0	1.85e-21	1.000	220.5	1.92e-21	1.000
221.0	2.01e-21	1.000	221.5	2.11e-21	1.000	222.0	2.23e-21	1.000	222.5	2.33e-21	1.000	223.0	2.48e-21	1.000
223.5	2.60e-21	1.000	224.0	2.74e-21	1.000	224.5	2.85e-21	1.000	225.0	3.04e-21	1.000	225.5	3.15e-21	1.000
226.0	3.33e-21	1.000	226.5	3.55e-21	1.000	227.0	3.73e-21	1.000	227.5	3.93e-21	1.000	228.0	4.11e-21	1.000
228.5	4.34e-21	1.000	229.0	4.56e-21	1.000	229.5	4.75e-21	1.000	230.0	5.01e-21	1.000	230.5	5.27e-21	1.000
231.0	5.53e-21	1.000	231.5	5.83e-21	1.000	232.0	6.15e-21	1.000	232.5	6.45e-21	1.000	233.0	6.73e-21	1.000
233.5	7.02e-21	1.000	234.0	7.42e-21	1.000	234.5	7.83e-21	1.000	235.0	8.11e-21	1.000	235.5	8.45e-21	1.000
236.0	8.82e-21	1.000	236.5	9.21e-21	1.000	237.0	9.65e-21	1.000	237.5	1.00e-20	1.000	238.0	1.05e-20	1.000
238.5	1.10e-20	1.000	239.0	1.15e-20	1.000	239.5	1.20e-20	1.000	240.0	1.23e-20	1.000	240.5	1.28e-20	1.000
241.0	1.32e-20	1.000	241.5	1.38e-20	1.000	242.0	1.44e-20	1.000	242.5	1.50e-20	1.000	243.0	1.57e-20	1.000
243.5	1.63e-20	1.000	244.0	1.68e-20	1.000	244.5	1.75e-20	1.000	245.0	1.81e-20	1.000	245.5	1.88e-20	1.000
246.0	1.96e-20	1.000	246.5	2.03e-20	1.000	247.0	2.11e-20	1.000	247.5	2.19e-20	1.000	248.0	2.25e-20	1.000
248.5	2.33e-20	1.000	249.0	2.40e-20	1.000	249.5	2.48e-20	1.000	250.0	2.56e-20	1.000	250.5	2.64e-20	1.000

WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY
251.0	2.73e-20	1.000	251.5	2.81e-20	1.000	252.0	2.88e-20	1.000	252.5	2.98e-20	1.000	253.0	3.07e-20	1.000
253.5	3.16e-20	1.000	254.0	3.25e-20	1.000	254.5	3.34e-20	1.000	255.0	3.43e-20	1.000	255.5	3.51e-20	1.000
256.0	3.59e-20	1.000	256.5	3.67e-20	1.000	257.0	3.75e-20	1.000	257.5	3.84e-20	1.000	258.0	3.94e-20	1.000
258.5	4.03e-20	1.000	259.0	4.13e-20	1.000	259.5	4.22e-20	1.000	260.0	4.28e-20	1.000	260.5	4.33e-20	1.000
261.0	4.41e-20	1.000	261.5	4.49e-20	1.000	262.0	4.57e-20	1.000	262.5	4.65e-20	1.000	263.0	4.72e-20	1.000
263.5	4.78e-20	1.000	264.0	4.85e-20	1.000	264.5	4.92e-20	1.000	265.0	4.99e-20	1.000	265.5	5.04e-20	1.000
266.0	5.12e-20	1.000	266.5	5.22e-20	1.000	267.0	5.28e-20	1.000	267.5	5.34e-20	1.000	268.0	5.41e-20	1.000
268.5	5.46e-20	1.000	269.0	5.51e-20	1.000	269.5	5.55e-20	1.000	270.0	5.59e-20	1.000	270.5	5.63e-20	1.000
271.0	5.66e-20	1.000	271.5	5.70e-20	1.000	272.0	5.74e-20	1.000	272.5	5.78e-20	1.000	273.0	5.81e-20	1.000
273.5	5.86e-20	1.000	274.0	5.90e-20	1.000	274.5	5.93e-20	1.000	275.0	5.96e-20	1.000	275.5	5.97e-20	1.000
276.0	5.98e-20	1.000	276.5	5.98e-20	1.000	277.0	5.99e-20	1.000	277.5	5.99e-20	1.000	278.0	5.98e-20	1.000
278.5	5.96e-20	1.000	279.0	5.96e-20	1.000	279.5	5.95e-20	1.000	280.0	5.94e-20	1.000	280.5	5.92e-20	1.000
281.0	5.90e-20	1.000	281.5	5.88e-20	1.000	282.0	5.86e-20	1.000	282.5	5.83e-20	1.000	283.0	5.79e-20	1.000
283.5	5.75e-20	1.000	284.0	5.71e-20	1.000	284.5	5.67e-20	1.000	285.0	5.61e-20	1.000	285.5	5.56e-20	1.000
286.0	5.51e-20	1.000	286.5	5.45e-20	1.000	287.0	5.41e-20	1.000	287.5	5.37e-20	1.000	288.0	5.33e-20	1.000
288.5	5.27e-20	1.000	289.0	5.21e-20	1.000	289.5	5.15e-20	1.000	290.0	5.08e-20	1.000	290.5	4.99e-20	1.000
291.0	4.89e-20	1.000	291.5	4.82e-20	1.000	292.0	4.73e-20	1.000	292.5	4.62e-20	1.000	293.0	4.53e-20	1.000
293.5	4.41e-20	1.000	294.0	4.32e-20	1.000	294.5	4.23e-20	1.000	295.0	4.15e-20	1.000	295.5	4.11e-20	1.000
296.0	4.01e-20	1.000	296.5	3.94e-20	1.000	297.0	3.88e-20	1.000	297.5	3.77e-20	1.000	298.0	3.69e-20	1.000
298.5	3.63e-20	1.000	299.0	3.54e-20	1.000	299.5	3.46e-20	1.000	300.0	3.36e-20	1.000	300.5	3.24e-20	1.000
301.0	3.16e-20	1.000	301.5	3.06e-20	1.000	302.0	2.95e-20	1.000	302.5	2.82e-20	1.000	303.0	2.70e-20	1.000
303.5	2.59e-20	1.000	304.0	2.49e-20	1.000	304.5	2.42e-20	1.000	305.0	2.34e-20	1.000	305.5	2.28e-20	1.000
306.0	2.19e-20	1.000	306.5	2.11e-20	1.000	307.0	2.04e-20	1.000	307.5	1.93e-20	1.000	308.0	1.88e-20	1.000
308.5	1.80e-20	1.000	309.0	1.73e-20	1.000	309.5	1.66e-20	1.000	310.0	1.58e-20	1.000	310.5	1.48e-20	1.000
311.0	1.42e-20	1.000	311.5	1.34e-20	1.000	312.0	1.26e-20	1.000	312.5	1.17e-20	1.000	313.0	1.13e-20	1.000
313.5	1.08e-20	1.000	314.0	1.04e-20	1.000	314.5	9.69e-21	1.000	315.0	8.91e-21	1.000	315.5	8.61e-21	1.000
316.0	7.88e-21	1.000	316.5	7.25e-21	1.000	317.0	6.92e-21	1.000	317.5	6.43e-21	1.000	318.0	6.07e-21	1.000
318.5	5.64e-21	1.000	319.0	5.19e-21	1.000	319.5	4.66e-21	1.000	320.0	4.36e-21	1.000	320.5	3.95e-21	1.000
321.0	3.64e-21	1.000	321.5	3.38e-21	1.000	322.0	3.17e-21	1.000	322.5	2.80e-21	1.000	323.0	2.62e-21	1.000
323.5	2.29e-21	1.000	324.0	2.13e-21	1.000	324.5	1.93e-21	1.000	325.0	1.70e-21	1.000	325.5	1.58e-21	1.000
326.0	1.48e-21	1.000	326.5	1.24e-21	1.000	327.0	1.20e-21	1.000	327.5	1.04e-21	1.000	328.0	9.51e-22	1.000
328.5	8.44e-22	1.000	329.0	7.26e-22	1.000	329.5	6.70e-22	1.000	330.0	6.08e-22	1.000	330.5	5.15e-22	1.000
331.0	4.56e-22	1.000	331.5	4.13e-22	1.000	332.0	3.56e-22	1.000	332.5	3.30e-22	1.000	333.0	2.97e-22	1.000
333.5	2.67e-22	1.000	334.0	2.46e-22	1.000	334.5	2.21e-22	1.000	335.0	1.93e-22	1.000	335.5	1.56e-22	1.000
336.0	1.47e-22	1.000	336.5	1.37e-22	1.000	337.0	1.27e-22	1.000	337.5	1.19e-22	1.000	338.0	1.09e-22	1.000
338.5	1.01e-22	1.000	339.0	9.09e-23	1.000	339.5	8.22e-23	1.000	340.0	7.66e-23	1.000	340.5	7.43e-23	1.000
341.0	6.83e-23	1.000	341.5	6.72e-23	1.000	342.0	6.04e-23	1.000	342.5	4.78e-23	1.000	343.0	0.00e+00	1.000
COOH														
210.0	3.12e-19	1.000	215.0	2.09e-19	1.000	220.0	1.54e-19	1.000	225.0	1.22e-19	1.000	230.0	9.62e-20	1.000
235.0	7.61e-20	1.000	240.0	6.05e-20	1.000	245.0	4.88e-20	1.000	250.0	3.98e-20	1.000	255.0	3.23e-20	1.000
260.0	2.56e-20	1.000	265.0	2.11e-20	1.000	270.0	1.70e-20	1.000	275.0	1.39e-20	1.000	280.0	1.09e-20	1.000
285.0	8.63e-21	1.000	290.0	6.91e-21	1.000	295.0	5.51e-21	1.000	300.0	4.13e-21	1.000	305.0	3.13e-21	1.000
310.0	2.39e-21	1.000	315.0	1.82e-21	1.000	320.0	1.37e-21	1.000	325.0	1.05e-21	1.000	330.0	7.90e-22	1.000
335.0	6.10e-22	1.000	340.0	4.70e-22	1.000	345.0	3.50e-22	1.000	350.0	2.70e-22	1.000	355.0	2.10e-22	1.000
360.0	1.60e-22	1.000	365.0	1.20e-22	1.000	370.0	0.00e+00	1.000						
GLY_R														
230.0	2.87e-21	1.000	235.0	2.87e-21	1.000	240.0	4.30e-21	1.000	245.0	5.73e-21	1.000	250.0	8.60e-21	1.000
255.0	1.15e-20	1.000	260.0	1.43e-20	1.000	265.0	1.86e-20	1.000	270.0	2.29e-20	1.000	275.0	2.58e-20	1.000
280.0	2.87e-20	1.000	285.0	3.30e-20	1.000	290.0	3.15e-20	1.000	295.0	3.30e-20	1.000	300.0	3.58e-20	1.000
305.0	2.72e-20	1.000	310.0	2.72e-20	1.000	312.5	2.87e-20	1.000	315.0	2.29e-20	1.000	320.0	1.43e-20	1.000
325.0	1.15e-20	1.000	327.5	1.43e-20	1.000	330.0	1.15e-20	1.000	335.0	2.87e-21	1.000	340.0	0.00e+00	1.000
345.0	0.00e+00	1.000	350.0	0.00e+00	1.000	355.0	0.00e+00	1.000	360.0	2.29e-21	1.000	365.0	2.87e-21	1.000
370.0	8.03e-21	1.000	375.0	1.00e-20	1.000	380.0	1.72e-20	0.972	382.0	1.58e-20	0.855	384.0	1.49e-20	0.737

WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY
386.0	1.49e-20	0.619	388.0	2.87e-20	0.502	390.0	3.15e-20	0.384	391.0	3.24e-20	0.326	392.0	3.04e-20	0.267
393.0	2.23e-20	0.208	394.0	2.63e-20	0.149	395.0	3.04e-20	0.090	396.0	2.63e-20	0.032	397.0	2.43e-20	0.000
398.0	3.24e-20	0.000	399.0	3.04e-20	0.000	400.0	2.84e-20	0.000	401.0	3.24e-20	0.000	402.0	4.46e-20	0.000
403.0	5.27e-20	0.000	404.0	4.26e-20	0.000	405.0	3.04e-20	0.000	406.0	3.04e-20	0.000	407.0	2.84e-20	0.000
408.0	2.43e-20	0.000	409.0	2.84e-20	0.000	410.0	6.08e-20	0.000	411.0	5.07e-20	0.000	411.5	6.08e-20	0.000
412.0	4.86e-20	0.000	413.0	8.31e-20	0.000	413.5	6.48e-20	0.000	414.0	7.50e-20	0.000	414.5	8.11e-20	0.000
415.0	8.11e-20	0.000	415.5	6.89e-20	0.000	416.0	4.26e-20	0.000	417.0	4.86e-20	0.000	418.0	5.88e-20	0.000

GLY_ABS

230.0	2.87e-21	1.000	235.0	2.87e-21	1.000	240.0	4.30e-21	1.000	245.0	5.73e-21	1.000	250.0	8.60e-21	1.000
255.0	1.15e-20	1.000	260.0	1.43e-20	1.000	265.0	1.86e-20	1.000	270.0	2.29e-20	1.000	275.0	2.58e-20	1.000
280.0	2.87e-20	1.000	285.0	3.30e-20	1.000	290.0	3.15e-20	1.000	295.0	3.30e-20	1.000	300.0	3.58e-20	1.000
305.0	2.72e-20	1.000	310.0	2.72e-20	1.000	312.5	2.87e-20	1.000	315.0	2.29e-20	1.000	320.0	1.43e-20	1.000
325.0	1.15e-20	1.000	327.5	1.43e-20	1.000	330.0	1.15e-20	1.000	335.0	2.87e-21	1.000	340.0	0.00e+00	1.000
355.0	0.00e+00	1.000	360.0	2.29e-21	1.000	365.0	2.87e-21	1.000	370.0	8.03e-21	1.000	375.0	1.00e-20	1.000
380.0	1.72e-20	1.000	382.0	1.58e-20	1.000	384.0	1.49e-20	1.000	386.0	1.49e-20	1.000	388.0	2.87e-20	1.000
390.0	3.15e-20	1.000	391.0	3.24e-20	1.000	392.0	3.04e-20	1.000	393.0	2.23e-20	1.000	394.0	2.63e-20	1.000
395.0	3.04e-20	1.000	396.0	2.63e-20	1.000	397.0	2.43e-20	1.000	398.0	3.24e-20	1.000	399.0	3.04e-20	1.000
400.0	2.84e-20	1.000	401.0	3.24e-20	1.000	402.0	4.46e-20	1.000	403.0	5.27e-20	1.000	404.0	4.26e-20	1.000
405.0	3.04e-20	1.000	406.0	3.04e-20	1.000	407.0	2.84e-20	1.000	408.0	2.43e-20	1.000	409.0	2.84e-20	1.000
410.0	6.08e-20	1.000	411.0	5.07e-20	1.000	411.5	6.08e-20	1.000	412.0	4.86e-20	1.000	413.0	8.31e-20	1.000
413.5	6.48e-20	1.000	414.0	7.50e-20	1.000	414.5	8.11e-20	1.000	415.0	8.11e-20	1.000	415.5	6.89e-20	1.000
416.0	4.26e-20	1.000	417.0	4.86e-20	1.000	418.0	5.88e-20	1.000	419.0	6.69e-20	1.000	420.0	3.85e-20	1.000
421.0	5.67e-20	1.000	421.5	4.46e-20	1.000	422.0	5.27e-20	1.000	422.5	1.05e-19	1.000	423.0	8.51e-20	1.000
424.0	6.08e-20	1.000	425.0	7.29e-20	1.000	426.0	1.18e-19	1.000	426.5	1.30e-19	1.000	427.0	1.07e-19	1.000
428.0	1.66e-19	1.000	429.0	4.05e-20	1.000	430.0	5.07e-20	1.000	431.0	4.86e-20	1.000	432.0	4.05e-20	1.000
433.0	3.65e-20	1.000	434.0	4.05e-20	1.000	434.5	6.08e-20	1.000	435.0	5.07e-20	1.000	436.0	8.11e-20	1.000
436.5	1.13e-19	1.000	437.0	5.27e-20	1.000	438.0	1.01e-19	1.000	438.5	1.38e-19	1.000	439.0	7.70e-20	1.000
440.0	2.47e-19	1.000	441.0	8.11e-20	1.000	442.0	6.08e-20	1.000	443.0	7.50e-20	1.000	444.0	9.32e-20	1.000
445.0	1.13e-19	1.000	446.0	5.27e-20	1.000	447.0	2.43e-20	1.000	448.0	2.84e-20	1.000	449.0	3.85e-20	1.000
450.0	6.08e-20	1.000	451.0	1.09e-19	1.000	451.5	9.32e-20	1.000	452.0	1.22e-19	1.000	453.0	2.39e-19	1.000
454.0	1.70e-19	1.000	455.0	3.40e-19	1.000	455.5	4.05e-19	1.000	456.0	1.01e-19	1.000	457.0	1.62e-20	1.000
458.0	1.22e-20	1.000	458.5	1.42e-20	1.000	459.0	4.05e-21	1.000	460.0	4.05e-21	1.000	460.5	6.08e-21	1.000
461.0	2.03e-21	1.000	462.0	0.00e+00	1.000									

MGLY_ADJ

219.0	9.84e-21	1.000	219.5	1.04e-20	1.000	220.0	1.06e-20	1.000	220.5	1.11e-20	1.000	221.0	1.15e-20	1.000
221.5	1.18e-20	1.000	222.0	1.22e-20	1.000	222.5	1.24e-20	1.000	223.0	1.26e-20	1.000	223.5	1.26e-20	1.000
224.0	1.25e-20	1.000	224.5	1.24e-20	1.000	225.0	1.25e-20	1.000	225.5	1.27e-20	1.000	226.0	1.27e-20	1.000
226.5	1.29e-20	1.000	227.0	1.31e-20	1.000	227.5	1.32e-20	1.000	228.0	1.35e-20	1.000	228.5	1.37e-20	1.000
229.0	1.40e-20	1.000	229.5	1.42e-20	1.000	230.0	1.48e-20	1.000	230.5	1.53e-20	1.000	231.0	1.57e-20	1.000
231.5	1.59e-20	1.000	232.0	1.61e-20	1.000	232.5	1.62e-20	1.000	233.0	1.61e-20	1.000	233.5	1.68e-20	1.000
234.0	1.74e-20	1.000	234.5	1.80e-20	1.000	235.0	1.84e-20	1.000	235.5	1.87e-20	1.000	236.0	1.89e-20	1.000
236.5	1.91e-20	1.000	237.0	1.93e-20	1.000	237.5	1.94e-20	1.000	238.0	1.96e-20	1.000	238.5	1.96e-20	1.000
239.0	2.01e-20	1.000	239.5	2.04e-20	1.000	240.0	2.08e-20	1.000	240.5	2.10e-20	1.000	241.0	2.14e-20	1.000
241.5	2.16e-20	1.000	242.0	2.19e-20	1.000	242.5	2.20e-20	1.000	243.0	2.23e-20	1.000	243.5	2.26e-20	1.000
244.0	2.28e-20	1.000	244.5	2.29e-20	1.000	245.0	2.30e-20	1.000	245.5	2.32e-20	1.000	246.0	2.33e-20	1.000
246.5	2.35e-20	1.000	247.0	2.38e-20	1.000	247.5	2.41e-20	1.000	248.0	2.46e-20	1.000	248.5	2.51e-20	1.000
249.0	2.57e-20	1.000	249.5	2.61e-20	1.000	250.0	2.65e-20	1.000	250.5	2.67e-20	1.000	251.0	2.69e-20	1.000
251.5	2.69e-20	1.000	252.0	2.71e-20	1.000	252.5	2.72e-20	1.000	253.0	2.73e-20	1.000	253.5	2.74e-20	1.000
254.0	2.76e-20	1.000	254.5	2.78e-20	1.000	255.0	2.82e-20	1.000	255.5	2.87e-20	1.000	256.0	2.93e-20	1.000
256.5	2.98e-20	1.000	257.0	3.07e-20	1.000	257.5	3.12e-20	1.000	258.0	3.17e-20	1.000	258.5	3.21e-20	1.000
259.0	3.26e-20	1.000	259.5	3.28e-20	1.000	260.0	3.29e-20	1.000	260.5	3.31e-20	1.000	261.0	3.33e-20	1.000
261.5	3.34e-20	1.000	262.0	3.36e-20	1.000	262.5	3.38e-20	1.000	263.0	3.42e-20	1.000	263.5	3.44e-20	1.000
264.0	3.48e-20	1.000	264.5	3.54e-20	1.000	265.0	3.59e-20	1.000	265.5	3.65e-20	1.000	266.0	3.73e-20	1.000

WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY
266.5	3.80e-20	1.000	267.0	3.87e-20	1.000	267.5	3.95e-20	1.000	268.0	4.02e-20	1.000	268.5	4.08e-20	1.000
269.0	4.13e-20	1.000	269.5	4.17e-20	1.000	270.0	4.20e-20	1.000	270.5	4.22e-20	1.000	271.0	4.22e-20	1.000
271.5	4.22e-20	1.000	272.0	4.23e-20	1.000	272.5	4.24e-20	1.000	273.0	4.27e-20	1.000	273.5	4.29e-20	1.000
274.0	4.31e-20	1.000	274.5	4.33e-20	1.000	275.0	4.37e-20	1.000	275.5	4.42e-20	1.000	276.0	4.48e-20	1.000
276.5	4.56e-20	1.000	277.0	4.64e-20	1.000	277.5	4.71e-20	1.000	278.0	4.78e-20	1.000	278.5	4.83e-20	1.000
279.0	4.87e-20	1.000	279.5	4.90e-20	1.000	280.0	4.92e-20	1.000	280.5	4.93e-20	1.000	281.0	4.94e-20	1.000
281.5	4.92e-20	1.000	282.0	4.90e-20	1.000	282.5	4.86e-20	1.000	283.0	4.83e-20	1.000	283.5	4.79e-20	1.000
284.0	4.76e-20	1.000	284.5	4.72e-20	1.000	285.0	4.70e-20	1.000	285.5	4.68e-20	1.000	286.0	4.66e-20	1.000
286.5	4.65e-20	1.000	287.0	4.65e-20	1.000	287.5	4.68e-20	1.000	288.0	4.73e-20	1.000	288.5	4.78e-20	1.000
289.0	4.84e-20	1.000	289.5	4.89e-20	1.000	290.0	4.92e-20	1.000	290.5	4.92e-20	1.000	291.0	4.90e-20	1.000
291.5	4.86e-20	1.000	292.0	4.81e-20	1.000	292.5	4.75e-20	1.000	293.0	4.70e-20	1.000	293.5	4.65e-20	1.000
294.0	4.58e-20	1.000	294.5	4.48e-20	1.000	295.0	4.38e-20	1.000	295.5	4.27e-20	1.000	296.0	4.17e-20	1.000
296.5	4.07e-20	1.000	297.0	3.99e-20	1.000	297.5	3.94e-20	1.000	298.0	3.88e-20	1.000	298.5	3.82e-20	1.000
299.0	3.76e-20	1.000	299.5	3.72e-20	1.000	300.0	3.69e-20	1.000	300.5	3.68e-20	1.000	301.0	3.70e-20	1.000
301.5	3.72e-20	1.000	302.0	3.74e-20	1.000	302.5	3.74e-20	1.000	303.0	3.75e-20	1.000	303.5	3.71e-20	1.000
304.0	3.62e-20	1.000	304.5	3.51e-20	1.000	305.0	3.38e-20	1.000	305.5	3.25e-20	1.000	306.0	3.15e-20	1.000
306.5	3.04e-20	1.000	307.0	2.92e-20	1.000	307.5	2.80e-20	1.000	308.0	2.71e-20	1.000	308.5	2.63e-20	1.000
309.0	2.52e-20	1.000	309.5	2.43e-20	1.000	310.0	2.34e-20	1.000	310.5	2.25e-20	1.000	311.0	2.19e-20	1.000
311.5	2.12e-20	1.000	312.0	2.06e-20	1.000	312.5	2.02e-20	1.000	313.0	1.96e-20	1.000	313.5	1.92e-20	1.000
314.0	1.91e-20	1.000	314.5	1.88e-20	1.000	315.0	1.86e-20	1.000	315.5	1.85e-20	1.000	316.0	1.86e-20	1.000
316.5	1.87e-20	1.000	317.0	1.87e-20	1.000	317.5	1.87e-20	1.000	318.0	1.83e-20	1.000	318.5	1.75e-20	1.000
319.0	1.69e-20	1.000	319.5	1.60e-20	1.000	320.0	1.50e-20	1.000	320.5	1.41e-20	1.000	321.0	1.34e-20	1.000
321.5	1.27e-20	1.000	322.0	1.21e-20	1.000	322.5	1.18e-20	1.000	323.0	1.14e-20	1.000	323.5	1.08e-20	1.000
324.0	1.01e-20	1.000	324.5	9.62e-21	1.000	325.0	9.28e-21	1.000	325.5	8.75e-21	1.000	326.0	8.49e-21	1.000
326.5	8.21e-21	1.000	327.0	7.71e-21	1.000	327.5	7.38e-21	1.000	328.0	7.18e-21	1.000	328.5	6.86e-21	1.000
329.0	6.71e-21	1.000	329.5	6.63e-21	1.000	330.0	6.46e-21	1.000	330.5	6.29e-21	1.000	331.0	6.21e-21	1.000
331.5	6.18e-21	1.000	332.0	6.20e-21	1.000	332.5	5.49e-21	1.000	333.0	5.21e-21	1.000	333.5	5.38e-21	1.000
334.0	5.35e-21	1.000	334.5	5.04e-21	1.000	335.0	4.94e-21	1.000	335.5	4.90e-21	1.000	336.0	4.52e-21	1.000
336.5	4.26e-21	1.000	337.0	4.11e-21	1.000	337.5	3.76e-21	1.000	338.0	3.61e-21	1.000	338.5	3.58e-21	1.000
339.0	3.47e-21	1.000	339.5	3.32e-21	1.000	340.0	3.22e-21	1.000	340.5	3.10e-21	1.000	341.0	3.00e-21	1.000
341.5	2.94e-21	1.000	342.0	2.89e-21	1.000	342.5	2.86e-21	1.000	343.0	2.88e-21	1.000	343.5	2.88e-21	1.000
344.0	2.89e-21	0.992	344.5	2.91e-21	0.984	345.0	2.95e-21	0.976	345.5	3.00e-21	0.968	346.0	3.08e-21	0.960
346.5	3.18e-21	0.953	347.0	3.25e-21	0.945	347.5	3.30e-21	0.937	348.0	3.39e-21	0.929	348.5	3.51e-21	0.921
349.0	3.63e-21	0.913	349.5	3.73e-21	0.905	350.0	3.85e-21	0.897	350.5	3.99e-21	0.889	351.0	4.27e-21	0.881
351.5	4.47e-21	0.873	352.0	4.63e-21	0.865	352.5	4.78e-21	0.858	353.0	4.92e-21	0.850	353.5	5.07e-21	0.842
354.0	5.23e-21	0.834	354.5	5.39e-21	0.826	355.0	5.56e-21	0.818	355.5	5.77e-21	0.810	356.0	5.97e-21	0.802
356.5	6.15e-21	0.794	357.0	6.35e-21	0.786	357.5	6.56e-21	0.778	358.0	6.76e-21	0.770	358.5	6.95e-21	0.763
359.0	7.20e-21	0.755	359.5	7.44e-21	0.747	360.0	7.64e-21	0.739	360.5	7.89e-21	0.731	361.0	8.15e-21	0.723
361.5	8.43e-21	0.715	362.0	8.71e-21	0.707	362.5	9.02e-21	0.699	363.0	9.33e-21	0.691	363.5	9.65e-21	0.683
364.0	1.00e-20	0.675	364.5	1.04e-20	0.668	365.0	1.08e-20	0.660	365.5	1.11e-20	0.652	366.0	1.15e-20	0.644
366.5	1.19e-20	0.636	367.0	1.23e-20	0.628	367.5	1.27e-20	0.620	368.0	1.31e-20	0.612	368.5	1.35e-20	0.604
369.0	1.40e-20	0.596	369.5	1.44e-20	0.588	370.0	1.47e-20	0.580	370.5	1.51e-20	0.573	371.0	1.55e-20	0.565
371.5	1.59e-20	0.557	372.0	1.64e-20	0.549	372.5	1.70e-20	0.541	373.0	1.73e-20	0.533	373.5	1.77e-20	0.525
374.0	1.81e-20	0.517	374.5	1.86e-20	0.509	375.0	1.90e-20	0.501	375.5	1.96e-20	0.493	376.0	2.02e-20	0.486
376.5	2.06e-20	0.478	377.0	2.10e-20	0.470	377.5	2.14e-20	0.462	378.0	2.18e-20	0.454	378.5	2.24e-20	0.446
379.0	2.30e-20	0.438	379.5	2.37e-20	0.430	380.0	2.42e-20	0.422	380.5	2.47e-20	0.414	381.0	2.54e-20	0.406
381.5	2.62e-20	0.398	382.0	2.69e-20	0.391	382.5	2.79e-20	0.383	383.0	2.88e-20	0.375	383.5	2.96e-20	0.367
384.0	3.02e-20	0.359	384.5	3.10e-20	0.351	385.0	3.20e-20	0.343	385.5	3.29e-20	0.335	386.0	3.39e-20	0.327
386.5	3.51e-20	0.319	387.0	3.62e-20	0.311	387.5	3.69e-20	0.303	388.0	3.70e-20	0.296	388.5	3.77e-20	0.288
389.0	3.88e-20	0.280	389.5	3.97e-20	0.272	390.0	4.03e-20	0.264	390.5	4.12e-20	0.256	391.0	4.22e-20	0.248
391.5	4.29e-20	0.240	392.0	4.30e-20	0.232	392.5	4.38e-20	0.224	393.0	4.47e-20	0.216	393.5	4.55e-20	0.208
394.0	4.56e-20	0.201	394.5	4.59e-20	0.193	395.0	4.67e-20	0.185	395.5	4.80e-20	0.177	396.0	4.87e-20	0.169
396.5	4.96e-20	0.161	397.0	5.08e-20	0.153	397.5	5.19e-20	0.145	398.0	5.23e-20	0.137	398.5	5.39e-20	0.129
399.0	5.46e-20	0.121	399.5	5.54e-20	0.113	400.0	5.59e-20	0.106	400.5	5.77e-20	0.098	401.0	5.91e-20	0.090

WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY
401.5	5.99e-20	0.082	402.0	6.06e-20	0.074	402.5	6.20e-20	0.066	403.0	6.35e-20	0.058	403.5	6.52e-20	0.050
404.0	6.54e-20	0.042	404.5	6.64e-20	0.034	405.0	6.93e-20	0.026	405.5	7.15e-20	0.018	406.0	7.19e-20	0.011
406.5	7.32e-20	0.003	407.0	7.58e-20	0.000	407.5	7.88e-20	0.000	408.0	7.97e-20	0.000	408.5	7.91e-20	0.000
409.0	8.11e-20	0.000	409.5	8.41e-20	0.000	410.0	8.53e-20	0.000	410.5	8.59e-20	0.000	411.0	8.60e-20	0.000
411.5	8.80e-20	0.000	412.0	9.04e-20	0.000	412.5	9.45e-20	0.000	413.0	9.34e-20	0.000	413.5	9.37e-20	0.000
414.0	9.63e-20	0.000	414.5	9.71e-20	0.000	415.0	9.70e-20	0.000	415.5	9.65e-20	0.000	416.0	9.69e-20	0.000
416.5	9.89e-20	0.000	417.0	1.00e-19	0.000	417.5	1.02e-19	0.000	418.0	1.00e-19	0.000	418.5	1.02e-19	0.000
419.0	1.01e-19	0.000	419.5	1.01e-19	0.000	420.0	1.03e-19	0.000	420.5	1.01e-19	0.000	421.0	1.04e-19	0.000
BACL_ADJ														
230.0	1.30e-20	1.000	232.5	1.46e-20	1.000	235.0	1.68e-20	1.000	237.5	1.84e-20	1.000	240.0	2.16e-20	1.000
242.5	2.49e-20	1.000	245.0	2.65e-20	1.000	247.5	2.71e-20	1.000	250.0	3.03e-20	1.000	252.5	3.46e-20	1.000
255.0	3.46e-20	1.000	257.5	3.57e-20	1.000	260.0	3.95e-20	1.000	262.5	4.17e-20	1.000	265.0	4.17e-20	1.000
267.5	4.22e-20	1.000	270.0	4.60e-20	1.000	272.5	4.54e-20	1.000	275.0	4.33e-20	1.000	277.5	4.22e-20	1.000
280.0	4.44e-20	1.000	282.5	4.33e-20	1.000	285.0	3.90e-20	1.000	287.5	3.57e-20	1.000	290.0	3.25e-20	1.000
292.5	2.92e-20	1.000	295.0	2.60e-20	1.000	297.5	2.16e-20	1.000	300.0	1.79e-20	1.000	302.5	1.73e-20	1.000
305.0	1.46e-20	1.000	307.5	1.08e-20	1.000	310.0	9.20e-21	1.000	312.5	7.03e-21	1.000	315.0	6.49e-21	1.000
317.5	5.41e-21	1.000	320.0	5.41e-21	1.000	322.5	5.41e-21	1.000	325.0	4.33e-21	1.000	327.5	3.25e-21	1.000
330.0	3.79e-21	1.000	332.5	3.79e-21	1.000	335.0	4.33e-21	1.000	337.5	4.87e-21	1.000	340.0	5.41e-21	1.000
342.5	5.95e-21	1.000	345.0	6.49e-21	1.000	347.5	7.03e-21	1.000	350.0	8.12e-21	0.995	352.5	7.57e-21	0.960
355.0	9.20e-21	0.925	357.5	9.74e-21	0.890	360.0	1.08e-20	0.855	362.5	1.19e-20	0.820	365.0	1.41e-20	0.785
367.5	1.51e-20	0.750	370.0	1.79e-20	0.715	372.5	2.00e-20	0.680	375.0	2.11e-20	0.645	377.5	2.33e-20	0.610
380.0	2.60e-20	0.575	382.5	2.81e-20	0.540	385.0	3.14e-20	0.505	387.5	3.46e-20	0.470	390.0	3.90e-20	0.435
392.5	4.11e-20	0.399	395.0	4.33e-20	0.364	397.5	4.38e-20	0.329	400.0	4.65e-20	0.294	402.5	4.81e-20	0.259
405.0	5.19e-20	0.224	407.5	5.84e-20	0.189	410.0	6.06e-20	0.154	412.5	6.49e-20	0.119	415.0	6.92e-20	0.084
417.5	6.87e-20	0.049	420.0	6.82e-20	0.014	422.5	6.71e-20	0.000	425.0	6.49e-20	0.000	427.5	5.95e-20	0.000
430.0	5.73e-20	0.000	432.5	6.28e-20	0.000	435.0	6.01e-20	0.000	437.5	5.84e-20	0.000	440.0	5.95e-20	0.000
442.5	6.49e-20	0.000	445.0	5.95e-20	0.000	447.5	4.98e-20	0.000	450.0	3.79e-20	0.000	452.5	2.81e-20	0.000
455.0	1.73e-20	0.000	457.5	1.08e-20	0.000	460.0	5.41e-21	0.000	462.5	3.79e-21	0.000	465.0	2.16e-21	0.000
467.5	1.08e-21	0.000	470.0	1.08e-21	0.000	472.5	0.00e+00	0.000						
BZCHO														
299.0	1.78e-19	1.000	304.0	7.40e-20	1.000	306.0	6.91e-20	1.000	309.0	6.41e-20	1.000	313.0	6.91e-20	1.000
314.0	6.91e-20	1.000	318.0	6.41e-20	1.000	325.0	8.39e-20	1.000	332.0	7.65e-20	1.000	338.0	8.88e-20	1.000
342.0	8.88e-20	1.000	346.0	7.89e-20	1.000	349.0	7.89e-20	1.000	354.0	9.13e-20	1.000	355.0	8.14e-20	1.000
364.0	5.67e-20	1.000	368.0	6.66e-20	1.000	369.0	8.39e-20	1.000	370.0	8.39e-20	1.000	372.0	3.45e-20	1.000
374.0	3.21e-20	1.000	376.0	2.47e-20	1.000	377.0	2.47e-20	1.000	380.0	3.58e-20	1.000	382.0	9.90e-21	1.000
386.0	0.00e+00	1.000												
ACROLEIN														
250.0	1.80e-21	1.000	252.0	2.05e-21	1.000	253.0	2.20e-21	1.000	254.0	2.32e-21	1.000	255.0	2.45e-21	1.000
256.0	2.56e-21	1.000	257.0	2.65e-21	1.000	258.0	2.74e-21	1.000	259.0	2.83e-21	1.000	260.0	2.98e-21	1.000
261.0	3.24e-21	1.000	262.0	3.47e-21	1.000	263.0	3.58e-21	1.000	264.0	3.93e-21	1.000	265.0	4.67e-21	1.000
266.0	5.10e-21	1.000	267.0	5.38e-21	1.000	268.0	5.73e-21	1.000	269.0	6.13e-21	1.000	270.0	6.64e-21	1.000
271.0	7.20e-21	1.000	272.0	7.77e-21	1.000	273.0	8.37e-21	1.000	274.0	8.94e-21	1.000	275.0	9.55e-21	1.000
276.0	1.04e-20	1.000	277.0	1.12e-20	1.000	278.0	1.19e-20	1.000	279.0	1.27e-20	1.000	280.0	1.27e-20	1.000
281.0	1.26e-20	1.000	282.0	1.26e-20	1.000	283.0	1.28e-20	1.000	284.0	1.33e-20	1.000	285.0	1.38e-20	1.000
286.0	1.44e-20	1.000	287.0	1.50e-20	1.000	288.0	1.57e-20	1.000	289.0	1.63e-20	1.000	290.0	1.71e-20	1.000
291.0	1.78e-20	1.000	292.0	1.86e-20	1.000	293.0	1.95e-20	1.000	294.0	2.05e-20	1.000	295.0	2.15e-20	1.000
296.0	2.26e-20	1.000	297.0	2.37e-20	1.000	298.0	2.48e-20	1.000	299.0	2.60e-20	1.000	300.0	2.73e-20	1.000
301.0	2.85e-20	1.000	302.0	2.99e-20	1.000	303.0	3.13e-20	1.000	304.0	3.27e-20	1.000	305.0	3.39e-20	1.000
306.0	3.51e-20	1.000	307.0	3.63e-20	1.000	308.0	3.77e-20	1.000	309.0	3.91e-20	1.000	310.0	4.07e-20	1.000
311.0	4.25e-20	1.000	312.0	4.39e-20	1.000	313.0	4.44e-20	1.000	314.0	4.50e-20	1.000	315.0	4.59e-20	1.000
316.0	4.75e-20	1.000	317.0	4.90e-20	1.000	318.0	5.05e-20	1.000	319.0	5.19e-20	1.000	320.0	5.31e-20	1.000
321.0	5.43e-20	1.000	322.0	5.52e-20	1.000	323.0	5.60e-20	1.000	324.0	5.67e-20	1.000	325.0	5.67e-20	1.000

WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY
326.0	5.62e-20	1.000	327.0	5.63e-20	1.000	328.0	5.71e-20	1.000	329.0	5.76e-20	1.000	330.0	5.80e-20	1.000
331.0	5.95e-20	1.000	332.0	6.23e-20	1.000	333.0	6.39e-20	1.000	334.0	6.38e-20	1.000	335.0	6.24e-20	1.000
336.0	6.01e-20	1.000	337.0	5.79e-20	1.000	338.0	5.63e-20	1.000	339.0	5.56e-20	1.000	340.0	5.52e-20	1.000
341.0	5.54e-20	1.000	342.0	5.53e-20	1.000	343.0	5.47e-20	1.000	344.0	5.41e-20	1.000	345.0	5.40e-20	1.000
346.0	5.48e-20	1.000	347.0	5.90e-20	1.000	348.0	6.08e-20	1.000	349.0	6.00e-20	1.000	350.0	5.53e-20	1.000
351.0	5.03e-20	1.000	352.0	4.50e-20	1.000	353.0	4.03e-20	1.000	354.0	3.75e-20	1.000	355.0	3.55e-20	1.000
356.0	3.45e-20	1.000	357.0	3.46e-20	1.000	358.0	3.49e-20	1.000	359.0	3.41e-20	1.000	360.0	3.23e-20	1.000
361.0	2.95e-20	1.000	362.0	2.81e-20	1.000	363.0	2.91e-20	1.000	364.0	3.25e-20	1.000	365.0	3.54e-20	1.000
366.0	3.30e-20	1.000	367.0	2.78e-20	1.000	368.0	2.15e-20	1.000	369.0	1.59e-20	1.000	370.0	1.19e-20	1.000
371.0	8.99e-21	1.000	372.0	7.22e-21	1.000	373.0	5.86e-21	1.000	374.0	4.69e-21	1.000	375.0	3.72e-21	1.000
376.0	3.57e-21	1.000	377.0	3.55e-21	1.000	378.0	2.83e-21	1.000	379.0	1.69e-21	1.000	380.0	8.29e-24	1.000
381.0	0.00e+00	1.000												

IC3ONO2

185.0	1.79e-17	1.000	188.0	1.81e-17	1.000	190.0	1.79e-17	1.000	195.0	1.61e-17	1.000	200.0	1.26e-17	1.000
205.0	8.67e-18	1.000	210.0	4.98e-18	1.000	215.0	2.47e-18	1.000	220.0	1.17e-18	1.000	225.0	5.80e-19	1.000
230.0	3.10e-19	1.000	235.0	1.80e-19	1.000	240.0	1.10e-19	1.000	245.0	7.00e-20	1.000	250.0	5.70e-20	1.000
255.0	5.20e-20	1.000	260.0	4.90e-20	1.000	265.0	4.60e-20	1.000	270.0	4.10e-20	1.000	275.0	3.60e-20	1.000
280.0	2.90e-20	1.000	285.0	2.30e-20	1.000	290.0	1.70e-20	1.000	295.0	1.20e-20	1.000	300.0	8.10e-21	1.000
305.0	5.20e-21	1.000	310.0	3.20e-21	1.000	315.0	1.90e-21	1.000	320.0	1.10e-21	1.000	325.0	6.10e-22	1.000
330.0	3.70e-22	1.000	335.0	0.00e+00	1.000									

MGLY_ABS

219.0	9.84e-21	1.000	219.5	1.04e-20	1.000	220.0	1.06e-20	1.000	220.5	1.11e-20	1.000	221.0	1.15e-20	1.000
221.5	1.18e-20	1.000	222.0	1.22e-20	1.000	222.5	1.24e-20	1.000	223.0	1.26e-20	1.000	223.5	1.26e-20	1.000
224.0	1.25e-20	1.000	224.5	1.24e-20	1.000	225.0	1.25e-20	1.000	225.5	1.27e-20	1.000	226.0	1.27e-20	1.000
226.5	1.29e-20	1.000	227.0	1.31e-20	1.000	227.5	1.32e-20	1.000	228.0	1.35e-20	1.000	228.5	1.37e-20	1.000
229.0	1.40e-20	1.000	229.5	1.42e-20	1.000	230.0	1.48e-20	1.000	230.5	1.53e-20	1.000	231.0	1.57e-20	1.000
231.5	1.59e-20	1.000	232.0	1.61e-20	1.000	232.5	1.62e-20	1.000	233.0	1.61e-20	1.000	233.5	1.68e-20	1.000
234.0	1.74e-20	1.000	234.5	1.80e-20	1.000	235.0	1.84e-20	1.000	235.5	1.87e-20	1.000	236.0	1.89e-20	1.000
236.5	1.91e-20	1.000	237.0	1.93e-20	1.000	237.5	1.94e-20	1.000	238.0	1.96e-20	1.000	238.5	1.96e-20	1.000
239.0	2.01e-20	1.000	239.5	2.04e-20	1.000	240.0	2.08e-20	1.000	240.5	2.10e-20	1.000	241.0	2.14e-20	1.000
241.5	2.16e-20	1.000	242.0	2.19e-20	1.000	242.5	2.20e-20	1.000	243.0	2.23e-20	1.000	243.5	2.26e-20	1.000
244.0	2.28e-20	1.000	244.5	2.29e-20	1.000	245.0	2.30e-20	1.000	245.5	2.32e-20	1.000	246.0	2.33e-20	1.000
246.5	2.35e-20	1.000	247.0	2.38e-20	1.000	247.5	2.41e-20	1.000	248.0	2.46e-20	1.000	248.5	2.51e-20	1.000
249.0	2.57e-20	1.000	249.5	2.61e-20	1.000	250.0	2.65e-20	1.000	250.5	2.67e-20	1.000	251.0	2.69e-20	1.000
251.5	2.69e-20	1.000	252.0	2.71e-20	1.000	252.5	2.72e-20	1.000	253.0	2.73e-20	1.000	253.5	2.74e-20	1.000
254.0	2.76e-20	1.000	254.5	2.78e-20	1.000	255.0	2.82e-20	1.000	255.5	2.87e-20	1.000	256.0	2.93e-20	1.000
256.5	2.98e-20	1.000	257.0	3.07e-20	1.000	257.5	3.12e-20	1.000	258.0	3.17e-20	1.000	258.5	3.21e-20	1.000
259.0	3.26e-20	1.000	259.5	3.28e-20	1.000	260.0	3.29e-20	1.000	260.5	3.31e-20	1.000	261.0	3.33e-20	1.000
261.5	3.34e-20	1.000	262.0	3.36e-20	1.000	262.5	3.38e-20	1.000	263.0	3.42e-20	1.000	263.5	3.44e-20	1.000
264.0	3.48e-20	1.000	264.5	3.54e-20	1.000	265.0	3.59e-20	1.000	265.5	3.65e-20	1.000	266.0	3.73e-20	1.000
266.5	3.80e-20	1.000	267.0	3.87e-20	1.000	267.5	3.95e-20	1.000	268.0	4.02e-20	1.000	268.5	4.08e-20	1.000
269.0	4.13e-20	1.000	269.5	4.17e-20	1.000	270.0	4.20e-20	1.000	270.5	4.22e-20	1.000	271.0	4.22e-20	1.000
271.5	4.22e-20	1.000	272.0	4.23e-20	1.000	272.5	4.24e-20	1.000	273.0	4.27e-20	1.000	273.5	4.29e-20	1.000
274.0	4.31e-20	1.000	274.5	4.33e-20	1.000	275.0	4.37e-20	1.000	275.5	4.42e-20	1.000	276.0	4.48e-20	1.000
276.5	4.56e-20	1.000	277.0	4.64e-20	1.000	277.5	4.71e-20	1.000	278.0	4.78e-20	1.000	278.5	4.83e-20	1.000
279.0	4.87e-20	1.000	279.5	4.90e-20	1.000	280.0	4.92e-20	1.000	280.5	4.93e-20	1.000	281.0	4.94e-20	1.000
281.5	4.92e-20	1.000	282.0	4.90e-20	1.000	282.5	4.86e-20	1.000	283.0	4.83e-20	1.000	283.5	4.79e-20	1.000
284.0	4.76e-20	1.000	284.5	4.72e-20	1.000	285.0	4.70e-20	1.000	285.5	4.68e-20	1.000	286.0	4.66e-20	1.000
286.5	4.65e-20	1.000	287.0	4.65e-20	1.000	287.5	4.68e-20	1.000	288.0	4.73e-20	1.000	288.5	4.78e-20	1.000
289.0	4.84e-20	1.000	289.5	4.89e-20	1.000	290.0	4.92e-20	1.000	290.5	4.92e-20	1.000	291.0	4.90e-20	1.000
291.5	4.86e-20	1.000	292.0	4.81e-20	1.000	292.5	4.75e-20	1.000	293.0	4.70e-20	1.000	293.5	4.65e-20	1.000
294.0	4.58e-20	1.000	294.5	4.48e-20	1.000	295.0	4.38e-20	1.000	295.5	4.27e-20	1.000	296.0	4.17e-20	1.000
296.5	4.07e-20	1.000	297.0	3.99e-20	1.000	297.5	3.94e-20	1.000	298.0	3.88e-20	1.000	298.5	3.82e-20	1.000

WL (nm)	Abs (cm^2)	QY (nm)	WL	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY
299.0	3.76e-20	1.000	299.5	3.72e-20	1.000	300.0	3.69e-20	1.000	300.5	3.68e-20	1.000	301.0	3.70e-20	1.000
301.5	3.72e-20	1.000	302.0	3.74e-20	1.000	302.5	3.74e-20	1.000	303.0	3.75e-20	1.000	303.5	3.71e-20	1.000
304.0	3.62e-20	1.000	304.5	3.51e-20	1.000	305.0	3.38e-20	1.000	305.5	3.25e-20	1.000	306.0	3.15e-20	1.000
306.5	3.04e-20	1.000	307.0	2.92e-20	1.000	307.5	2.80e-20	1.000	308.0	2.71e-20	1.000	308.5	2.63e-20	1.000
309.0	2.52e-20	1.000	309.5	2.43e-20	1.000	310.0	2.34e-20	1.000	310.5	2.25e-20	1.000	311.0	2.19e-20	1.000
311.5	2.12e-20	1.000	312.0	2.06e-20	1.000	312.5	2.02e-20	1.000	313.0	1.96e-20	1.000	313.5	1.92e-20	1.000
314.0	1.91e-20	1.000	314.5	1.88e-20	1.000	315.0	1.86e-20	1.000	315.5	1.85e-20	1.000	316.0	1.86e-20	1.000
316.5	1.87e-20	1.000	317.0	1.87e-20	1.000	317.5	1.87e-20	1.000	318.0	1.83e-20	1.000	318.5	1.75e-20	1.000
319.0	1.69e-20	1.000	319.5	1.60e-20	1.000	320.0	1.50e-20	1.000	320.5	1.41e-20	1.000	321.0	1.34e-20	1.000
321.5	1.27e-20	1.000	322.0	1.21e-20	1.000	322.5	1.18e-20	1.000	323.0	1.14e-20	1.000	323.5	1.08e-20	1.000
324.0	1.01e-20	1.000	324.5	9.62e-21	1.000	325.0	9.28e-21	1.000	325.5	8.75e-21	1.000	326.0	8.49e-21	1.000
326.5	8.21e-21	1.000	327.0	7.71e-21	1.000	327.5	7.38e-21	1.000	328.0	7.18e-21	1.000	328.5	6.86e-21	1.000
329.0	6.71e-21	1.000	329.5	6.63e-21	1.000	330.0	6.46e-21	1.000	330.5	6.29e-21	1.000	331.0	6.21e-21	1.000
331.5	6.18e-21	1.000	332.0	6.20e-21	1.000	332.5	5.49e-21	1.000	333.0	5.21e-21	1.000	333.5	5.38e-21	1.000
334.0	5.35e-21	1.000	334.5	5.04e-21	1.000	335.0	4.94e-21	1.000	335.5	4.90e-21	1.000	336.0	4.52e-21	1.000
336.5	4.26e-21	1.000	337.0	4.11e-21	1.000	337.5	3.76e-21	1.000	338.0	3.61e-21	1.000	338.5	3.58e-21	1.000
339.0	3.47e-21	1.000	339.5	3.32e-21	1.000	340.0	3.22e-21	1.000	340.5	3.10e-21	1.000	341.0	3.00e-21	1.000
341.5	2.94e-21	1.000	342.0	2.89e-21	1.000	342.5	2.86e-21	1.000	343.0	2.88e-21	1.000	343.5	2.88e-21	1.000
344.0	2.89e-21	1.000	344.5	2.91e-21	1.000	345.0	2.95e-21	1.000	345.5	3.00e-21	1.000	346.0	3.08e-21	1.000
346.5	3.18e-21	1.000	347.0	3.25e-21	1.000	347.5	3.30e-21	1.000	348.0	3.39e-21	1.000	348.5	3.51e-21	1.000
349.0	3.63e-21	1.000	349.5	3.73e-21	1.000	350.0	3.85e-21	1.000	350.5	3.99e-21	1.000	351.0	4.27e-21	1.000
351.5	4.47e-21	1.000	352.0	4.63e-21	1.000	352.5	4.78e-21	1.000	353.0	4.92e-21	1.000	353.5	5.07e-21	1.000
354.0	5.23e-21	1.000	354.5	5.39e-21	1.000	355.0	5.56e-21	1.000	355.5	5.77e-21	1.000	356.0	5.97e-21	1.000
356.5	6.15e-21	1.000	357.0	6.35e-21	1.000	357.5	6.56e-21	1.000	358.0	6.76e-21	1.000	358.5	6.95e-21	1.000
359.0	7.20e-21	1.000	359.5	7.44e-21	1.000	360.0	7.64e-21	1.000	360.5	7.89e-21	1.000	361.0	8.15e-21	1.000
361.5	8.43e-21	1.000	362.0	8.71e-21	1.000	362.5	9.02e-21	1.000	363.0	9.33e-21	1.000	363.5	9.65e-21	1.000
364.0	1.00e-20	1.000	364.5	1.04e-20	1.000	365.0	1.08e-20	1.000	365.5	1.11e-20	1.000	366.0	1.15e-20	1.000
366.5	1.19e-20	1.000	367.0	1.23e-20	1.000	367.5	1.27e-20	1.000	368.0	1.31e-20	1.000	368.5	1.35e-20	1.000
369.0	1.40e-20	1.000	369.5	1.44e-20	1.000	370.0	1.47e-20	1.000	370.5	1.51e-20	1.000	371.0	1.55e-20	1.000
371.5	1.59e-20	1.000	372.0	1.64e-20	1.000	372.5	1.70e-20	1.000	373.0	1.73e-20	1.000	373.5	1.77e-20	1.000
374.0	1.81e-20	1.000	374.5	1.86e-20	1.000	375.0	1.90e-20	1.000	375.5	1.96e-20	1.000	376.0	2.02e-20	1.000
376.5	2.06e-20	1.000	377.0	2.10e-20	1.000	377.5	2.14e-20	1.000	378.0	2.18e-20	1.000	378.5	2.24e-20	1.000
379.0	2.30e-20	1.000	379.5	2.37e-20	1.000	380.0	2.42e-20	1.000	380.5	2.47e-20	1.000	381.0	2.54e-20	1.000
381.5	2.62e-20	1.000	382.0	2.69e-20	1.000	382.5	2.79e-20	1.000	383.0	2.88e-20	1.000	383.5	2.96e-20	1.000
384.0	3.02e-20	1.000	384.5	3.10e-20	1.000	385.0	3.20e-20	1.000	385.5	3.29e-20	1.000	386.0	3.39e-20	1.000
386.5	3.51e-20	1.000	387.0	3.62e-20	1.000	387.5	3.69e-20	1.000	388.0	3.70e-20	1.000	388.5	3.77e-20	1.000
389.0	3.88e-20	1.000	389.5	3.97e-20	1.000	390.0	4.03e-20	1.000	390.5	4.12e-20	1.000	391.0	4.22e-20	1.000
391.5	4.29e-20	1.000	392.0	4.30e-20	1.000	392.5	4.38e-20	1.000	393.0	4.47e-20	1.000	393.5	4.55e-20	1.000
394.0	4.56e-20	1.000	394.5	4.59e-20	1.000	395.0	4.67e-20	1.000	395.5	4.80e-20	1.000	396.0	4.87e-20	1.000
396.5	4.96e-20	1.000	397.0	5.08e-20	1.000	397.5	5.19e-20	1.000	398.0	5.23e-20	1.000	398.5	5.39e-20	1.000
399.0	5.46e-20	1.000	399.5	5.54e-20	1.000	400.0	5.59e-20	1.000	400.5	5.77e-20	1.000	401.0	5.91e-20	1.000
401.5	5.99e-20	1.000	402.0	6.06e-20	1.000	402.5	6.20e-20	1.000	403.0	6.35e-20	1.000	403.5	6.52e-20	1.000
404.0	6.54e-20	1.000	404.5	6.64e-20	1.000	405.0	6.93e-20	1.000	405.5	7.15e-20	1.000	406.0	7.19e-20	1.000
406.5	7.32e-20	1.000	407.0	7.58e-20	1.000	407.5	7.88e-20	1.000	408.0	7.97e-20	1.000	408.5	7.91e-20	1.000
409.0	8.11e-20	1.000	409.5	8.41e-20	1.000	410.0	8.53e-20	1.000	410.5	8.59e-20	1.000	411.0	8.60e-20	1.000
411.5	8.80e-20	1.000	412.0	9.04e-20	1.000	412.5	9.45e-20	1.000	413.0	9.34e-20	1.000	413.5	9.37e-20	1.000
414.0	9.63e-20	1.000	414.5	9.71e-20	1.000	415.0	9.70e-20	1.000	415.5	9.65e-20	1.000	416.0	9.69e-20	1.000
416.5	9.89e-20	1.000	417.0	1.00e-19	1.000	417.5	1.02e-19	1.000	418.0	1.00e-19	1.000	418.5	1.02e-19	1.000
419.0	1.01e-19	1.000	419.5	1.01e-19	1.000	420.0	1.03e-19	1.000	420.5	1.01e-19	1.000	421.0	1.04e-19	1.000
421.5	1.05e-19	1.000	422.0	1.06e-19	1.000	422.5	1.04e-19	1.000	423.0	1.05e-19	1.000	423.5	1.05e-19	1.000
424.0	1.01e-19	1.000	424.5	1.01e-19	1.000	425.0	1.05e-19	1.000	425.5	1.03e-19	1.000	426.0	1.02e-19	1.000
426.5	1.01e-19	1.000	427.0	9.77e-20	1.000	427.5	9.81e-20	1.000	428.0	1.00e-19	1.000	428.5	1.02e-19	1.000
429.0	9.89e-20	1.000	429.5	9.85e-20	1.000	430.0	1.04e-19	1.000	430.5	1.08e-19	1.000	431.0	1.05e-19	1.000
431.5	1.02e-19	1.000	432.0	9.64e-20	1.000	432.5	1.01e-19	1.000	433.0	1.06e-19	1.000	433.5	1.09e-19	1.000

WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY	WL (nm)	Abs (cm^2)	QY
434.0	1.04e-19	1.000	434.5	1.03e-19	1.000	435.0	1.07e-19	1.000	435.5	1.16e-19	1.000	436.0	1.09e-19	1.000
436.5	1.11e-19	1.000	437.0	9.81e-20	1.000	437.5	9.71e-20	1.000	438.0	1.06e-19	1.000	438.5	1.16e-19	1.000
439.0	1.08e-19	1.000	439.5	1.05e-19	1.000	440.0	9.70e-20	1.000	440.5	1.01e-19	1.000	441.0	1.04e-19	1.000
441.5	1.07e-19	1.000	442.0	1.02e-19	1.000	442.5	9.68e-20	1.000	443.0	1.00e-19	1.000	443.5	1.14e-19	1.000
444.0	1.13e-19	1.000	444.5	1.03e-19	1.000	445.0	9.74e-20	1.000	445.5	8.46e-20	1.000	446.0	8.70e-20	1.000
446.5	9.97e-20	1.000	447.0	1.01e-19	1.000	447.5	9.15e-20	1.000	448.0	9.41e-20	1.000	448.5	8.99e-20	1.000
449.0	1.10e-19	1.000	449.5	9.12e-20	1.000	450.0	8.56e-20	1.000	450.5	8.28e-20	1.000	451.0	6.15e-20	1.000
451.5	5.56e-20	1.000	452.0	6.47e-20	1.000	452.5	7.27e-20	1.000	453.0	5.75e-20	1.000	453.5	5.08e-20	1.000
454.0	4.38e-20	1.000	454.5	3.81e-20	1.000	455.0	3.61e-20	1.000	455.5	3.61e-20	1.000	456.0	3.13e-20	1.000
456.5	2.72e-20	1.000	457.0	2.44e-20	1.000	457.5	2.22e-20	1.000	458.0	1.82e-20	1.000	458.5	1.43e-20	1.000
459.0	1.32e-20	1.000	459.5	1.05e-20	1.000	460.0	8.95e-21	1.000	460.5	8.90e-21	1.000	461.0	7.94e-21	1.000
461.5	7.04e-21	1.000	462.0	6.46e-21	1.000	462.5	5.63e-21	1.000	463.0	4.78e-21	1.000	463.5	3.94e-21	1.000
464.0	3.26e-21	1.000	464.5	2.97e-21	1.000	465.0	2.65e-21	1.000	465.5	2.46e-21	1.000	466.0	2.27e-21	1.000
466.5	2.08e-21	1.000	467.0	1.86e-21	1.000	467.5	1.76e-21	1.000	468.0	1.60e-21	1.000	468.5	1.44e-21	1.000
469.0	1.34e-21	1.000	469.5	1.20e-21	1.000	470.0	1.07e-21	1.000	470.5	1.02e-21	1.000	471.0	9.92e-22	1.000
471.5	9.97e-22	1.000	472.0	8.87e-22	1.000	472.5	8.27e-22	1.000	473.0	7.76e-22	1.000	473.5	7.15e-22	1.000
474.0	6.71e-22	1.000	474.5	6.67e-22	1.000	475.0	6.10e-22	1.000	475.5	6.17e-22	1.000	476.0	5.54e-22	1.000
476.5	5.22e-22	1.000	477.0	5.10e-22	1.000	477.5	5.17e-22	1.000	478.0	4.80e-22	1.000	478.5	4.71e-22	1.000
479.0	4.60e-22	1.000	479.5	4.35e-22	1.000	480.0	3.90e-22	1.000	480.5	3.71e-22	1.000	481.0	3.62e-22	1.000
481.5	3.52e-22	1.000	482.0	3.05e-22	1.000	482.5	3.05e-22	1.000	483.0	2.86e-22	1.000	483.5	2.53e-22	1.000
484.0	2.75e-22	1.000	484.5	2.59e-22	1.000	485.0	2.47e-22	1.000	485.5	2.36e-22	1.000	486.0	2.12e-22	1.000
486.5	1.89e-22	1.000	487.0	1.93e-22	1.000	487.5	1.86e-22	1.000	488.0	1.82e-22	1.000	488.5	1.75e-22	1.000
489.0	1.74e-22	1.000	489.5	1.72e-22	1.000	490.0	1.66e-22	1.000	490.5	1.75e-22	1.000	491.0	1.54e-22	1.000
491.5	1.74e-22	1.000	492.0	1.63e-22	1.000	492.5	1.53e-22	1.000	493.0	1.52e-22	1.000	493.5	5.85e-23	1.000
494.0	0.00e+00	1.000												

- Reactions of O^3P with O_3 and NO, which were omitted from the previous mechanism, are now included. These are believed to be negligible under most atmospheric conditions, but may not be in some high concentration experiments.

- The rate constant used for the "homogeneous" portion of the N_2O_5 hydrolysis reaction was decreased from 1 x 10^{-21} cm^3 $molec^{-1}$ s^{-1} to 2.6 x 10^{-22} cm^3 $molec^{-1}$ s^{-1}, based on the data of Mentel et al (1996). Note that this reaction may be primarily heterogeneous in nature, and the appropriate rate constant to use in atmospheric simulations is uncertain. However, the rate constant we use is not inconsistent with the IUPAC (Atkinson et al, 1997b) recommendation that the gas-phase rate constant is less than 2 x 10^{-21} cm^3 $molec^{-1}$ s^{-1}.

- The rate constant for OH + NO for 1 atmosphere and 300K increased by over a factor of 1.5, based on the NASA (1997) recommendation for the high pressure rate constant. The IUPAC (Atkinson et al, 1997a) recommendations is to use an even higher high pressure rate constant, but that recommendation is not used because the NASA value is more consistent with measurements made under near-atmospheric conditions.

- There is a significant discrepancy between the NASA (1997) and IUPAC (Atkinson et al, 1997a) recommendation concerning the important OH + NO_2 reaction. Again, the NASA recommendation is preferred because it is more consistent with measurements made under near-atmospheric conditions. [The rate parameters actually used are those that will be in the update to the NASA (1977) evaluation (Golden, private communication, 1999).] The high k_∞ recommended by IUPAC is based on very high pressure data in helium, and may be artifacts due to the contribution of a second reaction channel, involving HOONO formation, becoming important at higher pressures (Golden, personal communication, 1998). The value used in the current mechanism is about 20% lower than that used in the previous version. Given the importance of this reaction as a radical termination and NO_x removal process, this change may have a non-negligible effect on model simulations.

- The reaction of OH with HONO, which was omitted in the previous mechanism because of its low importance in ambient simulations, is now included. This reaction can be important in simulations of experiments with HONO added as a radical source, which may be useful for assessing some aspects of VOC reactivity (unpublished results from this laboratory).

- A second photolysis channel for HONO, forming H. + NO_2, was added based on the IUPAC (Atkinson et al, 1997) recommendations. This channel is calculated to occur ~10% of the time under atmospheric conditions.

- The reaction of OH with NO_3, omitted from the previous mechanism, is now included. The possibility that it may be non-negligible under some nighttime conditions or in some dark experiments has not been ruled out.

- The rate constant for the reaction of HO_2 with NO_3 was increased based on recent laboratory data of Mellouki et al (1993).

- The reaction of NO_3 with itself, which may be non-negligible under some nighttime conditions (Stockwell et al, 1997) is now included.

The effects of these changes on model simulations have not been evaluated. It is expected the ~20% change in the OH + NO_2 may be the most important in terms of predictions of ozone formation, and in the model simulations of the environmental chamber experiments used to evaluate the mechanism, as discussed in Section III. However some of the changes concerning NO_3 reactions may have non-negligible effects on nighttime simulations. As indicated above, a number of changes were added that are

not expected to influence ambient simulations, but which may be important in simulations of experiments that may be useful for evaluating other aspects of the mechanism. Since including these reactions did not add new species to the model, the impact of these reactions in terms of computational burden in airshed models should be minor.

2. Representation of Radical Species

The approaches used to represent the various types of radical species formed in the atmosphere are discussed in this section. As with the previous mechanism, most of the inorganic and a few of the organic radicals are represented explicitly, but most of the organic radicals are either lumped or not explicitly represented in the model. In particular, rapidly-reacting organic radicals which either react in only one way or whose reactions do not depend on other reacting species are replaced by the set of products they form, and most other radicals are either lumped or represented using a limited number of chemical "operators". The various approaches employed are discussed in this section.

With regard to computational impacts of radical species incorporated in the model, a distinction is made between *active* species and species where the *steady state* approximation can be employed. Active species are model species whose concentrations need to be calculated by the solver software by integrating their rates of change, and which must be transported in multi-cell model simulations. Steady state species are model species (usually representing rapidly reacting radical or chemical operators representing radicals) for which the steady state approximation can be employed. In that approximation, the concentration of the species is calculated at each time step assuming that the instantaneous rate of formation is equal to the rate of destruction. This means that the species does not need to be transported or integrated by the model software, saving computer time and memory in multi-cell simulations. This approximation can appropriately be used by species such as alkyl and alkoxy radicals that always react rapidly with O_2 or have rapid unimolecular reactions, and is implicitly used when a radical is removed in the model by replacing it with the compound(s) it forms. However, experience has shown that it cannot be used for peroxy or NO_3 radicals, since their loss processes can become slow compared to their rates of change under low NO_x conditions or at nighttime. In addition because of limitations in the mechanism compiling software used in this work [and also implemented in the FCM version of the UAM (Kumar et al, 1995) and the CALGRID model (??)], the steady state approximation cannot be used for species that react with themselves, other steady state species, or whose instantaneous concentrations cannot be calculated from the active species concentrations in a stepwise manner (Carter, 1988). Because of the latter restriction, the steady state approximation cannot be used for OH radicals when the mechanism is implemented with this software, though probably it is not a bad approximation for this species.

a. Inorganic Radicals

Most of the inorganic radicals in the mechanism are represented explicitly, as shown on Table 1. The two exceptions are H atoms and $HOSO_2$ radicals, where the latter is formed in the reaction of OH with SO_2. H atoms are assumed to react exclusively and rapidly with O_2 to form HO_2, so any reaction that forms H atoms is represented as forming HO_2 instead. Likewise, $HOSO_2$ are assumed to react primarily with O_2 to form HO_2 and SO_3, so it is replaced by the HO_2 and sulfate (SULF) model species in the OH + SO_2 reaction. Table 1 indicates those radicals for which the steady state approximation can be used. Note that this approximation should not be used for HO_2 or NO_3 radicals because they may build up significantly in concentration at nighttime or in the absence of NO_x. It probably could be used for OH radicals, but is not because of limitations of software used to implement the mechanism, as indicated above.

b. Rapidly Reacting Radicals.

As with the previous versions of the mechanism, many rapidly radicals are removed from the mechanism by replacing them by the species they are assumed to rapidly form. Note that this can only be done for radicals where (1) the steady state approximation is appropriate, (2) the product(s) they ultimately form do not depend on any other reactants, and (3) the products they form also do not depend on reaction conditions (e.g., temperature) or the variation can be assumed to be insignificant for the conditions of the model application. The specific types of rapidly reacting radical substitution reactions used in this mechanism are as follows. Except as indicated, the substitution is due to an expected rapid reaction of the radical with O_2.

- HCO is replaced by HO_2 + CO.
- Based on product data for reactions of OH radicals with alcohols and other species, α-Hydroxy alkyl radicals are assumed to react with O_2 primarily by abstraction from the α-hydroxy rather than by addition. Therefore, such radicals are replaced by HO_2 + the corresponding carbonyl compound formed when it reacts with O_2. For example, $CH_3CH(\cdot)OH$ is replaced by CCHO + HO_2, where CCHO is the model species for acetaldehyde.
- α-Nitrato alkyl radicals are assumed to decompose unimolecularly to NO_2 + the corresponding carbonyl compound sufficiently rapidly that the decomposition will dominate over reaction with O_2. Therefore, such radicals are replaced by NO_2 + the corresponding carbonyl compound formed in the decomposition. For example, $CH_3CH(\cdot)NO_2$ is replaced by CCHO + NO_2.
- All other carbon-centered radicals, including acyl ($RCO\cdot$) and alkyl ($R\cdot$) are assumed to react entirely by O_2 addition. Therefore, these are replaced by the corresponding peroxy radical whenever they are formed.
- With the exception of t-butoxy (model species TBU-O·) and phenoxy (model species BZ-O·) radicals, which are represented explicitly in the mechanism, all alkoxy radicals are replaced by the set of products they are assumed to form when they react under atmospheric conditions. This would include reactions with O_2 and/or unimolecular reactions, as applicable. If the alkoxy radical has more than one reaction pathway that is assumed to be non-negligible, then non-integer stoichiometric coefficients are used for the products, as appropriate. The reactions of alkoxy radicals are discussed in Section ??.
- The Crigiee biradicals formed in the reactions of O_3 with alkenes are replaced by the set of products they are assumed to form when they react in the atmosphere, which includes stabilization as well as the various decomposition pathways. These reactions are probably temperature and pressure dependent, but since insufficient information is available to estimate these dependences, this is ignored. The reactions of Crigiee biradicals are discussed in the Section ??, in conjunction with the discussion of the general methods used for estimating O_3 + alkene reaction mechanisms.
- Stabilized Crigiee biradicals are replaced by the corresponding organic acid, on the assumption that their major fate under atmospheric conditions is reaction with H_2O to form the acid. The assumption that reaction with H_2O is the major fate of the biradicals is consistent with the rate constant ratios cited by Atkinson (1997a) for the reactions of $HCHO_2$ with H_2O, HCHO, CO, and NO_2. The mechanism for the reactions of stabilized $HCHO_2$ with water appear to be complex and may involve some formation of H_2O_2 or other peroxides, but based on the discussion of Atkinson (1999) we assume that acid formation is the major fate of all the stabilized Crigiee biradicals.

Note that branching ratios for some of the alkoxy radicals and the Crigiee biradicals may be temperature and pressure dependent, and this treatment ignores these dependencies. As discussed in Section ??, the alkoxy radical branching ratios are estimated for 300°C and 1 atmosphere total pressure, and thus they may not be optimum for simulations of high altitude or extreme temperature conditions. However, it should be pointed out that no other current mechanism represents these temperature and pressure dependences of product branching ratios, and doing so would require a significant increase in the complexity of the mechanism, or would require the model software to support temperature and pressure-varying parameters. Since no information is available concerning the temperature and pressure dependences of Crigiee biradical reactions, any representation of this in the model would be entirely speculative.

c. Explicitly Represented Organic Radicals

Most of the organic radical species are represented either by replacing them with the radicals or products they are expected to exclusively form, or by using the lumped peroxy radical species or "operators" as discussed in the following two sections. However, a few organic radical species are represented explicitly, either because their reactions are sufficiently different that they are not appropriately represented using the other approaches, or because it is believed representing them explicitly will improve the accuracy of the model sufficiently to make the added model species worthwhile. These are briefly discussed below.

Methyl Peroxy Radicals. In the previous mechanism, all peroxy radicals, including methyl peroxy, were represented using the general peroxy radical operators + the products they were expected to form, as discussed below. In this approach, the same organic products are assumed to be ultimately formed regardless of whether the radical reacts with NO, HO_2, or another peroxy radical. Although as discussed below this approach is still used for most of the higher peroxy radicals in this mechanism, in this mechanism methyl peroxy radicals ($CH_3OO\cdot$) are represented explicitly, using the model species C-O2·. Thus, the appropriate C_1 products are formed when it reacts with HO_2, itself, or other peroxy radicals, which are different than the formaldehyde formed when it reacts with NO. This allows for a more accurate representation of the reactions of at least this peroxy radical and gives this mechanism a level of detail approaching that of the RADM2 (Stockwell et al, 1990) or RACM (Stockwell et al, 1997) mechanisms in the way peroxy radical reactions are treated. As discussed by Carter and Lurmann (1990), the peroxy radical lumping approach used in the RADM2 mechanism appears to be somewhat less approximate than the lumping approach used in the previous SAPRC mechanisms.

Note that the reactions of peroxy radicals with NO_3 were not in the previous version of the mechanism. This reaction, which may be non-negligible at nighttime, was added based on the recommendations of the current evaluations (Atkinson et al, 1997a,b).

Acyl Peroxy Radicals. The previous mechanism used separate steady-state model species to represent acyl peroxy radicals (CCO-O2·), general lumped higher acyl peroxy radicals (C2CO-O2·), and the higher peroxy radicals formed from glyoxal (HCOCO-O2·) and benzaldehyde (BZCO-O2·). In addition, the model species (RCO3·) was used to compute the total concentration without using the steady state approximation, for the purpose of computing peroxy + peroxy reaction rates. The PAN analogues for these radicals (PAN, PPN, GPAN, and BZ-PAN) were also included in the mechanism as active species. In this mechanism, the acyl peroxy radical formed from glyoxal (and its PAN analogue) are removed by lumping them with the other higher general lumped peroxy radicals (or PAN analogues), the acyl peroxy radical (and PAN analogue) formed from methacrolein and other isoprene products are added, and the total acyl peroxy radical model species (RCO3·) is removed. The need for RCO3· is eliminated by treating all the acyl peroxy radical model species as active, and including all their cross

reactions. Although this requires more reactions and active species in the mechanism than the approach used previously, it gives a somewhat more accurate representation of the peroxy + peroxy reactions of these species, which can be important at nighttime, and eliminates the need to include a separate total peroxy radical operator as a co-product in every reaction forming such radicals.

T-Butoxy Radicals. As indicated above, most alkoxy radicals are not represented explicitly in the mechanism, but are replaced by the set of species they are assumed to form when they react. In the previous mechanism this was the case for all organic alkoxy radicals except for phenoxy (see below), and in particular, t-butoxy radicals were assumed to react exclusively by decomposition to acetone and methyl radicals. However, the decomposition of t-butoxy is believed to be relatively slow (see Table 2), and if NO_2 levels are sufficiently high then reaction with NO_2 may be non-negligible in high-NO_x scenarios or chamber experiments. In particular, the reaction of t-butoxy with NO_2 had to be included for the model to appropriately simulate results of incremental reactivity chamber experiments with isobutane (Carter et al, 1993a). Because the competition between decomposition and NO_2 depends on the NO_2 concentration, this requires that t-butoxy radicals be represented explicitly in the model. This is not necessary for most other alkoxy radicals, which can either react sufficiently rapidly with O_2, or have sufficiently rapid decomposition or isomerization pathways, that reaction with NO_2 can be neglected.

Phenoxy Radicals. Phenoxy radicals are represented explicitly in this and the previous mechanism because they are not expected to react with O_2 and have no known rapid decomposition pathway. In the presence of NO_x, the major fate of phenoxy radicals is believed to be reaction with NO_2, since it has no obvious unimolecular reaction route or mechanism for reaction with O_2. (Reaction with NO would be expected to form a nitrite that would rapidly photolyze to re-form NO and phenoxy.) Nitrophenol formation has generally been assumed in this reaction (e.g., see Atkinson, 1990; Carter, 1990), presumably via some rearrangement of an initially formed unstable adduct. However, based on lower than expected yields of Nitrophenol in NO3 + cresol and OH + benzaldehyde systems (Atkinson, 1994), this may be an oversimplification. In the absence of NO_x, the major fate of phenoxy is assumed to be reaction with HO_2, though the model also includes a slow unimolecular loss to account for situations where NO_2 or HO_2 may be low. Note that the phenoxy radical model species is used as a surrogate for substituted phenoxy radicals as well, except for lumped nitro-substituted phenoxy radicals, discussed below.

Nitro-Phenoxy Radicals. Although their reaction mechanisms are assumed to be the same as phenoxy radicals, the NO_2-substituted phenoxy radicals assumed to be formed from the reactions of NO_3 with phenols are represented separately. This is done to account for nitrogen balance, and because the dinitroaromatics expected to be formed in the reaction with NO_2 are expected to be either non-volatile or non-reactive, and are thus represented in the model as "lost nitrogen". This is the same representation as used in the previous mechanisms.

Formaldehyde + HO_2 Intermediate. The radical believed to be formed when HO_2 reacts with formaldehyde has to be represented explicitly because its subsequent fate is believed to be affected by NO levels, as shown on Table 2. The mechanism used is based on the IUPAC (Atkinson et al, 1999) recommendation, and is essentially the same as used in the previous mechanism.

d. Peroxy Radical Operators

Representation of peroxy radical reactions in mechanisms is complicated by the fact that a relatively large number of such radicals are formed even in condensed mechanisms, and they can react to a non-negligible extent with themselves and other peroxy radicals under some conditions. The approach employed in the Carter (1990) mechanism is to represent organic peroxy radicals with the set of

products they would ultimately form if they reacted fully in the presence of NO_x and sunlight, together with a set of chemical "operators" that represent their other effects on the system. A total peroxy radical operator (RO2·) is used to compute the total peroxy radical concentrations for the purpose of computing peroxy + peroxy radical reaction rates; this allows the steady-state approximation to be used for the other peroxy radical operators.

The approach used in this mechanism is similar, except that as indicated above it is not used for methyl peroxy because it is now represented explicitly, and also the total peroxy radical species (RO2·) is eliminated. Instead of the latter, all the peroxy radical operators are treated as active species, and the cross-reactions between the operators are included. The elimination of RO2· simplifies the representation of peroxy radical chemistry and reduces the total number of species in the mechanism, though at the expense of having a somewhat larger number of active species and peroxy + peroxy radical cross reactions. The number of peroxy radical operators used to represent organic nitrate formation was reduced to reduce the number of species and cross-reactions. The peroxy radical operators employed in this mechanism are summarized below.

RO2-R·. This operator represents the effect of peroxy radical reactions that ultimately cause one NO to NO2 conversion and formation of HO_2 when they react with NO. It is representing as having zero carbons. When this operator reacts with HO_2, it is represented as forming ROOH, the lumped higher hydroperoxide species. Unlike the previous mechanism (Carter, 1990), which used a zero-carbon lumped hydroperoxide operator (-OOH) to represent the effect of hydroperoxide photolysis to form radicals, in this mechanism the higher hydroperoxides are represented by a model species whose reactions are based on those estimated for n-propyl hydroperoxide. In other words, a lumped molecule approach is used rather than the lumped structure approach. Since the organic portion of the radicals already represented by the products formed if the radical reacted with NO (which is why the RO2-R· operators are zero carbon species), formation of the ROOH in the HO_2 reaction does not conserve carbon. To account for this, loss of three "lost carbon" (XC) species are included in this reaction to main carbon balance. Although this may appear to be a worse approximation than using a zero-carbon lumped structure species such as the -OOH in the previous mechanism, in fact for most radicals carbon is lost in the model when the peroxy reacts with NO (because of the use of relatively small products to represent most of the lumped products), so this tends to work towards compensating for that effect. Tracing the "lost carbon" (XC) levels in the model can be used to track the extent to which carbon is lost due to the way the product species are represented.

When this operator reacts with explicitly the represented radical species [i.e., NO_3, methyl peroxy, or any of the acyl peroxy species] the products formed are the same as would be formed if ethyl peroxy (CH_3CH_2OO·) reacted with those species, except that any C_2 organic products (acetaldehyde or ethanol) are removed, and if ethoxy radicals are formed, they are replaced by HO_2 (based on the fact that ethoxy can be represented as rapidly forming acetaldehyde + HO_2, with acetaldehyde removed). In other words, since the since RO2-R· does not represent the organic portions of the peroxy radicals, the organic products formed in its reactions are ignored. Note that it is assumed that in RO_2· + RO_2· reactions it is assumed that formation of 2 RO· + O_2 and disproportionation to an alcohol + a carbonyl + O_2 occur with equal probability, based on available data for higher peroxy radicals (Atkinson et al, 1999). In the case of reaction of methyl peroxy, it is assumed that the disproportionation forming methanol and that forming formaldehyde occur with equal probability.

R2O2·. This represents the effects of extra NO to NO_2 conversions caused by multi-step reaction mechanisms, as would occur, for example, in mechanisms involving alkoxy radical decompositions or isomerizations. Again, R2O2· is used so the model can account for the formation of RO_2, and [R2O2] is

used for the actual reactions of the operator. Unlike the RO2-R· and the other peroxy operators, this is not strictly speaking a radical species, and it is not represented as having any effect on the system except when it reacts with NO. This is because it does not react to form radical or radical sink species, and is only appropriately used in conjunction with RO2-R.

RO2-N·. This represents the reactions of peroxy radicals with NO forming organic nitrates of various types, which are all represented in the model by the 6-carbon lumped alkyl nitrate model species RNO3 (see Section 3.b). Note that in previous versions of the mechanisms two additional operators were used to represent these processes: RO2-XN· was used to represent peroxy radicals that reacted with NO to form relatively unreactive C_{3-} nitrates, and RO2-XN· was used to represent aromatic peroxy radicals that reacted with NO to form aromatic nitrates. In this mechanism RO2-XN· was removed because the amount of C_{3-} nitrate formation tends to be extremely small, and RO2-NP· was removed nitrate formation is assumed to be relatively minor for most aromatics. In addition, the reactions of the aromatic nitrates formed are so uncertain that representing them separately may not necessarily be any more accurate than lumping them with RNO3.

Since the RO2-N· operator is used to represent the organic nitrates formed when the peroxy radicals react with NO, it is represented as having the number of carbons of the nitrate it forms when it reacts with NO, and its reactions with species other than NO are based on this representation. The products are derived based on what is considered to be appropriate for a C_{6+} alkyl peroxy radical, since those tend to be the radicals that are the largest precursors to alkyl nitrates in atmospheric simulations. In addition, since primary radicals tend to be formed in lower relative yields from such higher molecular weight compounds than secondary or tertiary radicals (because the C-H bonds tend to be more labile), the carbonyl products are represented by ketone model species (MEK or PROD2), rather than by aldehydes. The specific products used are indicated in the footnotes to Table 2 for the various reactions.

RO_2 + RO_2 Reactions. Because the rate constants for peroxy + peroxy radical reactions can vary by orders of magnitude depending on the type of radical (e.g., Atkinson, 1997), the rate constant used for the peroxy + peroxy reactions of the peroxy radical operators must necessarily be very approximate. The value used for all these operators is based roughly on the range of rate constants for secondary peroxy radicals given by Atkinson (1997a) and Atkinson et al (1997b), and is 30 times higher than the 1×10^{-15} cm^3 $molec^{-1}$ s^{-1} value used in the previous mechanism (Carter 1990).

3. Reactions of Common Products

A total of 24 model species are used in this mechanism to represent the reactive organic product species, 11 of which are used for organic compounds that are represented explicitly, and 13 of which are used to represent groups of similar products using the "lumped molecule" approach. In most cases, the model species and mechanisms are not significantly different than in previous versions of the mechanisms, except that some of the rate constants were updated as indicated in footnotes to Table 2. Most of the updates for the C_{3-} products are based on IUPAC (Atkinson et al, 1997a, 1999) recommendations. The species used are summarized below.

a. Explicitly Represented and Lumped Molecule Products

Formaldehyde (HCHO) and Acetaldehyde (CCHO). The mechanisms for these two compounds are essentially the same as in the previous mechanism, except that some of the rate constants and absorption cross sections have been updated as recommended by IUPAC (Atkinson et al, 1997a, 1999). Note that this mechanism differs from most condensed mechanisms in that acetaldehyde is represented explicitly, with most higher aldehydes lumped with propionaldehyde, as discussed below.

The one exception is glycolaldehyde ($HOCH_2CHO$), which is expected to have a reactivity closer to acetaldehyde than propionaldehyde, and therefore is represented by acetaldehyde in this mechanism.

Propionaldehyde and Lumped Higher Aldehydes (RCHO). The reactions of the model species RCHO, which represents all C_{3+} aldehydes except glycolaldehyde, α-dicarbonyls, aromatic aldehydes, and acroleins, is based on the expected mechanism for propionaldehyde. Note that, based on structure-reactivity methods of Kwok and Atkinson (1995), as updated by Kwok et al (1996), approximately 4% of the reaction is estimated to occur by abstraction from the CH_2 group and ~1% at the methyl. The reactions of the radicals subsequently formed are derived using the general mechanism estimation methods, as discussed below. However, most of the OH reaction is analogous to the reaction of OH with acetaldehyde, forming RCO-O2·, the lumped higher acyl peroxy radical.

Acetone (ACET). Acetone is represented explicitly because it has significantly lower reactivity than other ketones, yet is sufficiently reactive that its reactivity is probably not negligible in long-range transport scenarios. Its mechanism is based on that discussed by Carter et al (1993b). Based on the data of Jenkin et al (1993), the $CH_3COCH_2O·$ radical is believed to primarily decompose to formaldehyde and $CH_3CO·$. The absorption cross sections and quantum yields are based on the IUPAC (Atkinson et al, 1997a), except that the reported quantum yields at 230 and 330 nm are believed to be high, and were corrected as discussed by Carter et al (1993b) and the footnotes to Reaction K3HV on Table 2. Note that the data of Carter et al (1993b) indicate that these quantum yields, even after adjustment, tend to slightly overpredict the reactivity of acetone in indoor and outdoor chamber experiments (see Section ?? for a discussion of the results of the evaluation of the mechanism against chamber data).

Methyl Ethyl Ketone and Lumped Lower Reactivity Ketones (MEK). This model species is used to represent ketones and other reactive oxygenated product species whose OH radical rate constant is between 5×10^{-13} and 5×10^{-12} cm^3 $molec^{-1}$ s^{-1}. Note that this is different from previous versions of the SAPRC mechanism, where MEK was used for all higher non-aldehyde, non-aromatic oxygenated products that were more reactive than acetone. The MEK mechanism is based on that derived for methyl ethyl ketone using the general mechanism estimation methods discussed below, the IUPAC recommended OH rate constant (Atkinson et al, 1999) and absorption cross sections provided by Moortgat (private communication, 1996). The overall photolysis quantum yield was derived by fits to some UNC chamber experiments as discussed by Carter et al (1986), but give reactivity predictions that are consistent with recent chamber experiments in our laboratory (see Section ?? and Carter et al, 1999a).

Methanol (MEOH). In previous SAPRC mechanisms methanol in emissions was represented as an assigned parameter detailed model species, which permitted it to be represented explicitly or lumped with other compounds, depending on the model application. However, this approach does not permit representing formation of methanol as a reaction product. In this mechanism methanol is assigned an explicit model species in order to permit its formation of a product in no-NO_x reactions of methyl peroxy reaction. These reactions, and the subsequent reactions of methanol so formed, may be non-negligible in some long-range transport scenarios. Since methanol is potentially important in emissions, most model applications would probably use a separate model species for it in any case. Indeed, methanol is now represented explicitly even in some condensed models such as expanded Carbon Bond IV (e.g., Carter, 1994b and references therein). The mechanism is based on IUPAC (Atkinson et al, 1997a, 1999) recommendations.

Methyl Hydroperoxide (COOH) and Lumped Higher Peroxides (ROOH). In previous SAPRC mechanisms, the hydroperoxide species formed in peroxy + HO_2 reactions were represented by a

single "lumped structure" model species "-OOH", combined with the organic products formed in the peroxy + NO reactions. In this mechanism, for more accurate representation of low-NO_x chemistry, for regional or long-range transport simulations, methyl hydroperoxide is represented explicitly, and the other hydroperoxides are represented using a separate model species (ROOH) using the "lumped molecule" approach. In the case of methyl hydroperoxide, the OH reaction is assumed to occur at both the methyl and OOH positions as recommended by IUPAC (Atkinson et al, 1997a, 1999), with the $\cdot CH_2OOH$ radical formed in the former reaction being assumed to rapidly decompose to formaldehyde + OH. The absorption cross sections are also based on IUPAC recommendations, with unit quantum yields assumed, and with the reaction assuming to proceed entirely by breaking the weak O-O bond.

The reactions of the lumped higher hydroperoxide (ROOH) are based on the estimated mechanism for n-propyl hydroperoxide. As discussed in footnotes to Table 2, the OH reaction is estimated to occur at the OOH group ~2/3 of the time, based on assuming the same rate constant as the same reaction of methyl hydroperoxide. Most of the remainder of the reaction is assumed to occur at the 1-position, yielding an α-hydroperoxy radical which is assumed to rapidly decompose to propionaldehyde (RCHO) and OH. The photolysis is assumed to have the same rate and an analogous mechanism as methyl hydroperoxide.

Glyoxal (GLY). Glyoxal, which is formed in the reactions of most aromatics, acetylene, and some other species [including some isoprene oxidation products (Carter and Atkinson, 1996)], continues to be represented explicitly in this mechanism. Since it is less reactive than some other aromatic products it is often not represented in condensed mechanisms, but it is known to make an important contribution to the reactivity of acetylene (Carter et al, 1997c) and benzene (see Section ??) and its reactivity is not well approximated by other model species. On the hand, this mechanism is somewhat more condensed than previous detailed SAPRC mechanisms in that the acyl peroxy radical and PAN analogue predicted to be formed from the OH + glyoxal reaction [$HCO(CO)OO\cdot$ and $HCO(CO)OONO_2$)] are not represented explicitly, but are lumped with RCO-O2· and PAN2 (see below). The mechanism for the OH reaction is based on the data of Niki et al (1985) as discussed by IUPAC (Atkinson et al, 1997a).

The glyoxal absorption cross sections were the same as used previously (Plum et al, 1983), as recommended by the IUPAC evaluation (Atkinson et al, 1997a). However, the quantum yields were significantly revised based modeling of acetylene - NO_x and acetylene reactivity environmental chamber data (Carter et al, 1997c), as discussed in footnotes to Table 2. The model simulations of those chamber experiments were found to be highly sensitive to glyoxal absorption cross sections used in the mechanism, and no other reasonable adjustments to the mechanism would yield acceptable fits to the data (Carter et al, 1997c). Note that to fit the data quantum yields which are ~1.4 times higher than overall quantum yield reported by Plum et al (1983) for conditions of those experiments muse be used. Although use of acetylene reactivity data is a highly indirect way to obtain glyoxal quantum yields, we consider it to be a less uncertain way to estimate radical quantum yields then the data of Plum et al (1993), which uses a UV-poor light source, only measures rates of glyoxal decay. Clearly this is uncertain and direct measurements of glyoxal quantum yields as a function of wavelength are needed.

Methyl Glyoxal (MGLY) and Other Higher α-dicarbonyl aldehydes. Methyl glyoxal is formed in the reactions of methylbenzenes and from some carbonyl compounds is a highly reactive compound that can significantly affect the reactivity of compounds that form it. The MGLY model species is also used to represent other α-dicarbonyl aldehydes, such as ethylglyoxal, etc. However, unlike the SAPRC-97 mechanism of Carter et al (1997a), but like earlier versions of the mechanism (Carter, 1990, 1995; Carter et al, 1993b), it is not used in this version of the mechanism to represent any of the uncharacterized aromatic ring fragmentation products (see discussion of unknown aromatic fragmentation

products, below). The mechanism for the OH and NO_3 reactions are similar to those in the previous mechanism, with the latter reaction assumed to have the same rate constant and analogous mechanism as for acetaldehyde.

The IUPAC recommended (Atkinson et al, 1997a, 1999) absorption cross sections for methyl glyoxal are approximately a factor of 2 higher than the Plum et al (1983) values used in the previous mechanism. The current mechanism uses cross sections obtained from Moortgat (personal communication, 1996), which are consistent with the IUPAC recommendations but have higher resolution. Unit quantum yields were assumed in the low wavelength band ($\lambda \leq 340$ nm) and zero quantum yields were assumed for wavelengths above the cutoff of 421 nm, as determined by the thermochemistry. For the rest of the high wavelength regime, the quantum yield was assumed to decline linearly from unity at 344 nm to zero at a wavelength (407 nm) that was adjusted such that the calculated overall photolysis rates under the conditions of the experiments of Plum et al (1983) agreed with the experimentally measured values. (An analogous treatment was used in when deriving the quantum yields for glyoxal and biacetyl, though in the glyoxal case the adjustment was to fit the acetylene chamber data, as indicated above.) Note that this gives a different wavelength dependence than assumed in the previous mechanism, where a wavelength-dependent overall quantum yield was assumed for the entire high-wavelength band, including wavelengths above the high wavelength cutoff.

Biacetyl (BACL) and Other α-Dicarbonyl Ketones. Biacetyl or other α-dicarbonyl ketones are formed in significant yields from p-xylene, 1,2,4-trimethylbenzene and other o-dimethyl aromatics, and might be formed from the reactions of some carbonyl compounds. Biacetyl was not represented in previous versions of the mechanism, being in effect represented by methyl glyoxal. However, because its chemistry is in some ways quite different from methyl glyoxal (it reacts only slowly with OH, and its photolysis forms only PAN precursors), it was decided to represent it explicitly in this mechanism. The BACL model species is also used for other α-dicarbonyl ketones.

The reaction of biacetyl with OH radicals is ignored because the OH + biacetyl rate constant is probably not much different than that for acetone, making it a negligible loss process compared to photolysis. The photolysis is assumed to proceed via breaking the weak CO-CO bond, as shown on Table 2. The absorption cross sections used were those from Plum et al (1983), and the wavelength-dependence of the quantum yields were derived from the data of Plum et al (1983) in a manner exactly analogous to that discussed above for methyl glyoxal (see footnotes to Table 2).

Phenol (PHEN) and Cresols (CRES). Phenol is formed from the reactions of benzene and is represented as being formed in the subsequent reactions of aromatic ring-retaining products such as cresols or benzaldehydes, and cresols are formed in the reactions of the substituted aromatics. Cresol is used to represent phenolic products formed from all alkyl-substituted benzenes, while phenol is used to represent such products formed from benzene and naphthalene, as well as phenolic products formed in secondary reactions of cresols. The relatively rapid reactions of these compounds with NO_3 represents a NO_x sink in the aromatic mechanisms that largely explains their predicted tendency to inhibit O_3 under low NO_x conditions. Therefore, it is important that these model species be in the mechanism. . They are kept as separate model species because the reactions of cresols are assumed to involve some PAN (or PAN analogue) formation, while this is assumed not to be the case for phenol.

There are still inadequate data concerning the atmospheric reactions of these compounds and the products they form, and the highly parameterized mechanisms used in the previous versions of the SAPRC mechanisms are essentially unchanged in this version. The main consumption reactions are with OH and NO_3, and the rate constants used are those recommended by Atkinson (1994). The OH + cresol

mechanism is based on the highly parameterized mechanism derived by Carter (1990), but the version for this mechanism was reoptimized to fit the data from the single o-cresol - NO_x chamber experiment EC281 (Pitts et al, 1979; Carter et al, 1995d). The OH + phenol mechanism was derived by analogy with the resulting cresol mechanism. The NO_3 reactions are assumed to proceed via the formation of phenoxy radicals + HNO_3 (with the BZ-O· model species used for substituted as well as unsubstituted radicals, when then reacts as discussed above in Section 2.c. Note that although the mechanism for the NO_3 reaction (like that for the reaction with OH) is highly uncertain, it clearly must involve some sort of NO_x sink process in order for model simulations to fit chamber data for aromatics.

Nitrophenols (NPHE). The "nitrophenol" model species is used to represent whatever products are formed when phenoxy reacts with NO_2, which as indicated above is uncertain. It is assumed that the NO_2-substitution slows down the rate of reaction with OH radicals, and that its only significant consumption process is reaction with NO_3, for which it is assumed to have the same rate constant as phenol. This representation is unchanged from previous versions of the mechanism. Obviously this aspect of the mechanism is uncertain, but this representation appears to perform reasonably well in simulating effects of aromatics on peak O_3 yields, which are determined by NO_x-sink processes that are represented by the formation and reactions of NPHE.

Benzaldehyde (BALD) and Other Aromatic Aldehydes. Benzaldehyde, tolualdehydes and other aromatic aldehydes that are formed in a minor but non-negligible route in the reactions of OH with methylbenzenes are represented by the benzaldehyde (BALD) model species. Its OH and NO_3 reactions are assumed to be analogous to other aldehydes, except that separate model species (BZCO-O2· and BZ-PAN) are used to represent the acyl peroxy radical and PAN analogue formed. This is necessary because the reaction of the benzoyl peroxy radical with NO forms phenoxy radicals, which does not regenerate radicals like the radicals formed when the other acyl peroxy radicals react with NO.

The absorption cross sections for benzaldehyde (Majer et al, 1969) indicate that its photolysis can be significant if the quantum yield is sufficiently high. The quantum yields are unknown, but chamber data indicates that it is probably consumed to a non-negligible by photolysis, though the overall quantum yield is relatively low and the photolysis apparently does not involve significant radical formation, The overall quantum yield derived by Carter (1990) to fit SAPRC evacuable chamber data (Pitts et al, 1979) is retained in this mechanism. It was found to give reasonably good model simulations of benzaldehyde - NO_x experiments carried out in the CE-CERT Xenon Teflon Chamber (Carter et al, 1998a).

Methacrolein (METHACRO) and Methyl Vinyl Ketone (MVK). This version of the mechanism incorporates the "four product" isoprene mechanism (Carter, 1996) as part of the base mechanism, so it includes model species for methacrolein, MVK, and the lumped other isoprene products (ISOPROD). The mechanisms used for methacrolein and MVK are essentially the same as derived by Carter and Atkinson (1996), with some minor updates as indicated in footnotes to Table 2. The mechanisms were generated using the mechanism generation system discussed in Section ??, which incorporated most of the estimates and assignments of Carter and Atkinson (1996) for the reactions specific to the isoprene and isoprene product system. This resulted in some minor changes to yields of minor product in some reactions. In addition, because of these changes and changes to the overall base mechanism, the overall quantum yield for the methacrolein MVK photolysis was reoptimized, using the same procedures and data as discussed by Carter and Atkinson (1996). This resulted the overall quantum yield for methacrolein being increased by ~14%, while that for MVK was reduced by over a factor of ~5. The reason for this large change in the optimized MVK quantum yield is not clear, but it may be due to a

relatively low sensitivity of model simulation results to large changes in this parameter. (See Section ?? for results of model simulations of the methacrolein and MVK experiments.)

Methacrolein is also used to represent acrolein in reactions where acrolein is predicted to be formed as a product. This is to avoid adding a new model species to represent a relatively minor product in most ambient mixtures. However, as discussed in Section ??, this mechanism has a separate detailed model species for acrolein with mechanistic assignments appropriate for this compound, which can be used to more accurately represent acrolein when its reactivity is being assessed, or when emitted directly.

Lumped Isoprene Products (ISOPROD). The ISOPROD model species is used to represent reactive isoprene products other than methacrolein and MVK, and also to represent other unsaturated ketones or aldehydes (other than acrolein itself, which is represented by methacrolein) when formed in reactions of other VOCs. Its mechanism is based on the ISOPROD model species in the "four product" isoprene mechanism of Carter (1996), with some minor modifications as indicated in footnotes to Table 2. Its mechanism is derived from weighted averages of rate constants and parameters for a mixture of 30% hydroxymethacrolein and 23**a** % each cis-$HCOC(CH_3)$-$CHCH_2OH$, trans-$HCOC(CH_3)$-$CHCH_2OH$, and $HCOCH=C(CH_3)CH_2OH$. As with methacrolein and MVK, the mechanisms for these species were derived using the mechanism generation system discussed in Section ??, incorporating estimates and assignments of Carter and Atkinson (1996) where applicable. The mechanisms derived for these individual species are given with those for the other detailed model in Section ??.

b. Lumped Parameter Products

"Lumped parameter" species refer to model species whose mechanisms are derived by averaging rate constants and product yield parameters from a representative mixture of compounds that they are designed to represent. Although the previous versions of the SAPRC mechanism used this approach only for model species representing emitted VOCs, this mechanism also uses this approach for two of the lumped organic product species, as discussed below.

Lumped Higher Reactivity Non-Aldehyde Oxygenates (PROD2). This model species, which is new to this version of the mechanism, is used to represent ketones, alcohols, and other reactive non-aromatic and non-double-bond-containing oxygenated products whose rate constants are higher than 5×10^{-12} cm^3 $molec^{-1}$ s^{-1}. This was added because it was judged that many of the bi- or polyfunctional product species that were previously represented by MEK when they were formed as products are in fact much more reactive than MEK, at least in terms of their reaction rate with OH radicals. The reaction mechanism of PROD2 is based on averaging mechanisms derived for a representative set of product species as discussed below.

Lumped Organic Nitrate Products (RNO3). This model species is used to represent various organic nitrates (other than PAN or PAN analogues), primarily those formed in the reactions of peroxy radicals from NO. This is consumed primarily by reaction with OH radicals, but a slow photolysis, which may be non-negligible in long-range transport simulations, is also included in the mechanism. Unlike previous SAPRC mechanisms, RNO3 is also used to represent those formed from aromatic peroxy radicals with NO; previously the nitrophenol (NPHE) model species was used for this purpose. As indicated above, this change was made to avoid having to add the separate peroxy radical "operator" needed to support separate representation of aromatic nitrates, which are formed in relatively low yields and for which the appropriateness of the NPHE vs the RNO3 representation is unknown. The reaction mechanism of RNO3 is based on averaging mechanisms derived for a representative set of product species as discussed below.

Derivation of PROD2 and RNO3 Mechanisms. Although in principle the mechanisms for the lumped parameter product species can be derived for each emissions inventory in the manner used for the lumped parameter model species used for emitted VOCs (see Section ??), the necessary software to do this has not yet been developed. Instead, in this version of the mechanism the parameters are derived from sets of representative species representing products predicted to be formed from the reactions of the mixture of VOCs used as the "Base ROG" mixture in the atmospheric reactivity calculations (Carter, 1994a; see also Section ??), and are held fixed in the model simulations. The Base ROG mixture is used to represent reactive VOCs from all sources, and is derived from the "all city average" mixture derived by Jeffries et al (1989) from analysis of air quality data, with minor modifications as discussed by Carter (1994a,b)[1]. For the purpose of determining the contributions of the reactions of the compounds in the mixture to the formation of a lumped product, the contribution of each emitted VOC is weighed by the amount of each VOC that is estimated to react in a one-day scenario, multiplied by the yield of the lumped product used in the model for the reactions of the VOC. The amount reacted is obtained from the amount emitted multiplied by the "mechanistic reactivity" (Carter and Atkinson, 1989; Carter, 1994a), which is the fraction of the VOC estimated to react. The latter is obtained from mechanistic reactivities in the "averaged conditions" scenario where the NO_x inputs are adjusted to yield maximum peak ozone concentrations (the "MOIR" scenario)[2] (Carter, 1994; see tabulation in Section ?? for the values used). Tables 4 and 5 show the contributions of the reactions of various types of VOCs in the base ROG mixture to the formation of the RNO3 and PROD2 model species.

The set of compound that are represented by various model species can be calculated for those model species whose mechanisms can be derived using the mechanism generation/estimation system that is discussed in Section ??. For each of these compounds, the system generates the set of products that are predicted to be formed using a fully explicit mechanism for the reactions in the presence of NO_x, which are then used, together with the "lumping rules" discussed in Section ??, to determine the lumped product yields for the model. From this, the distribution of individual product VOCs represented by each lumped product model species can be determined, at least for the reactions of the VOCs whose mechanisms can be generated using this system. Although this system cannot generate mechanisms for aromatic compounds and terpenes, for which parameterized mechanisms must still be used, Tables 4 and 5 show that their contributions to PROD2 or RNO3 formation from the base ROG mixture is minor. In particular, reactions of aromatics and terpenes account for less than 6% of the PROD2 formation, and for less than 5% of the formation of RNO3 in one-day scenarios.

Table 6 and 7 show the 35 most important products predicted to be formed from the reactions of the VOCs in the base ROG mixture that are represented by PROD2 (Table 6) or RNO3 (Table 7). The tables also show the contribution of each product to the total of all products represented by PROD2 or RNO3, their OH radical rate constant and carbon numbers, and the average OH rate constant and carbon number for all the products, weighed by their molar contribution to the total. Note that no single compounds dominate the lists, and in the case of the organic nitrates the top 35 compounds account for less than half of the products formed that are represented by RNO3. Therefore, in both cases there is no obvious choice of a single "representative" or "typical" compound to use for lumped molecule representations.

---

[1] The complete mixture, indicating the specific detailed model species used to represent it in the model, is given in Section ??. See also Carter (1994b).

[2] The MOIR mechanistic reactivities are used because they are typical mechanistic reactivities in a wide range of scenarios. MIR mechanistic reactivities tend to be lower than in other scenarios because the relatively high NO_x levels tend to suppress radical levels.

Table 4. Contributions of various types of model species in the base ROG mixture to the formation of the PROD2 lumped product species.

VOC	Cont'n	VOC	Cont'n	VOC	Cont'n	VOC	Cont'n
N-C5	16.6%	1-HEXENE	2.5%	N-C11	0.8%	4-ME-C10	0.2%
N-C10	8.7%	3-ME-C6	2.2%	3-ME-C5	0.7%	1-PENTEN	0.2%
N-C6	6.6%	2-ME-C6	2.1%	36DM-C10	0.6%	3-ME-C10	0.2%
N-C7	6.2%	4-ME-C8	1.9%	1-C9E	0.6%	23-DM-C5	0.11%
Aromatics	5.6%	2-ME-C8	1.9%	24-DM-C5	0.6%	1-C10E	0.1%
24-DM-C6	4.6%	2-ME-C9	1.6%	ET-CYCC6	0.4%	1-PENTEN	0.1%
2-ME-C7	4.3%	4-ME-C9	1.6%	1-HEXENE	0.4%	2-ME-C5	0.1%
2-ME-C5	4.1%	26DM-C8	1.5%	5-ME-C11	0.3%	N-C13	0.1%
N-C8	3.8%	N-C12	1.4%	3-ME-C11	0.3%	36DM-C11	0.0%
N-C9	3.7%	1-HEPTEN	1.4%	1-OCTENE	0.3%	3-ME-C5	0.0%
CYCC6	2.9%	ME-CYCC6	1.1%	26DM-C9	0.2%	5-ME-C12	0.0%
4-ME-C7	2.9%	24-DM-C5	1.0%	ME-CYCC6	0.2%	3-ME-C12	0.0%
24-DM-C7	2.6%	3-ME-C6	0.9%	1-C11E	0.2%	22-DM-C4	0.0%

Table 5. Contributions of various types of model species in the base ROG mixture to the formation of the RNO3 lumped product species.

VOC	Cont'n	VOC	Cont'n	VOC	Cont'n	VOC	Cont'n
2-ME-C4	7.0%	Terpenes	1.5%	T-2-C6E	0.50%	CYC-HEXE	0.2%
N-C10	6.4%	2-ME-C9	1.4%	C-2-C6E	0.50%	1C5RCHO	0.2%
N-C4	5.8%	4-ME-C9	1.3%	1-C11E	0.46%	3M-1-BUT	0.2%
24-DM-C6	4.7%	2-ME-C8	1.3%	T-4-C9E	0.43%	3-ME-C10	0.2%
N-C5	4.4%	N-C12	1.3%	T-5-C11E	0.40%	4-ME-C10	0.2%
2-ME-C5	3.7%	4-ME-C8	1.3%	1-OCTENE	0.39%	MEK	0.1%
ME-CYCC5	3.5%	24-DM-C5	1.2%	1-PENTEN	0.36%	23-DM-C4	0.1%
Aromatics	3.0%	CYCC6	1.1%	T-2-BUTE	0.353%	2-ME-C3	0.1%
3-ME-C5	2.6%	C-2-PENT	1.1%	ME-CYCC6	0.3%	13-BUTDE	0.1%
26DM-C8	2.6%	T-2-PENT	1.1%	3-ME-C11	0.3%	2M-2-BUT	0.1%
N-C7	2.6%	CYCC5	1.1%	T-4-C8E	0.3%	2-ME-C5	0.1%
24-DM-C7	2.4%	1-C9E	1.0%	5-ME-C11	0.3%	3-ME-C5	0.1%
2-ME-C7	2.4%	PROPANE	1.0%	1-HEXENE	0.3%	N-C13	0.1%
4-ME-C7	2.3%	ISOBUTEN	1.0%	26DM-C9	0.3%	36DM-C11	0.0%
N-C9	2.3%	2-ME-C6	0.9%	22-DM-C4	0.3%	1-BUTENE	0.0%
3-ME-C6	2.2%	3-ME-C6	0.9%	C-2-BUTE	0.3%	C-2-BUTE	0.0%
1-HEXENE	2.1%	23-DM-C4	0.9%	T-2-C7E	0.2%	T-2-BUTE	0.0%
N-C8	2.0%	36DM-C10	0.7%	1C6RCHO	0.2%	1C4RCHO	0.0%
N-C6	1.9%	24-DM-C5	0.7%	1-BUTENE	0.2%	5-ME-C12	0.0%
ME-CYCC6	1.9%	N-C11	0.6%	1-C10E	0.2%	3-ME-C12	0.0%
23-DM-C5	1.7%	T-3-C7E	0.56%	1-PENTEN	0.2%		
1-HEPTEN	1.6%	ET-CYCC6	0.54%	T-4-C10E	0.2%		

Table 6. Product compounds predicted to be formed in the atmospheric reactions of compounds in the base ROG mixture that are represented by the PROD2 model species.

Cont'n [a]	kOH [b]	nC [c]	Model Species [d]	Product Structure [e]
	1.6e-11	7.14		Average of all Products
20.1%	9.6e-12	5	PROD2-1	CH3-CO-CH2-CH2-CH2-OH
4.9%	1.5e-11	6	PROD2-2	CH3-CO-CH2-CH(CH3)-CH2-OH
4.2%	2.7e-11	5		CH3-CH(OH)-CH2-CO-CH3
3.3%	1.4e-11	6		CH3-CH(OH)-CH2-CH2-CO-CH3
3.3%	6.4e-12	6		*CH2-CH2-CH2-CH2-CH2-CO-*
3.2%	1.1e-11	6		CH3-CH2-CO-CH2-CH2-CH2-OH
3.0%	1.7e-11	6		CH3-CH(OH)-CH2-CH2-CO-CH2-OH
2.8%	1.5e-11	7	PROD2-3	CH3-CH(OH)-CH2-CH2-CO-CH2-CH3
2.4%	1.7e-11	7		CH3-CH2-CH(OH)-CH2-CH2-CO-CH3
2.1%	2.3e-11	10		CH3-CH2-CH2-CH(OH)-CH2-CH2-CO-CH2-CH2-CH3
2.0%	2.1e-11	10		CH3-CH2-CH2-CH2-CH(OH)-CH2-CH2-CO-CH2-CH3
2.0%	7.1e-12	8		CH3-C(CH3)(OH)-CH2-CH2-CO-CH2-CH3
1.5%	2.1e-11	10		CH3-CH2-CH2-CH2-CH2-CH(OH)-CH2-CH2-CO-CH3
1.5%	2.0e-11	7		CH3-CH2-CH(OH)-CH2-CH2-CO-CH2-OH
1.4%	1.8e-11	8	PROD2-4	CH3-CH2-CH(OH)-CH2-CH2-CO-CH2-CH3
1.3%	2.4e-11	10		CH3-CH2-CH(OH)-CH2-CH2-CO-CH2-CH2-CH2-CH3
1.3%	6.0e-12	7		CH3-C(CH3)(OH)-CH2-CH2-CO-CH3
1.3%	1.4e-11	7		CH3-CH2-CH2-CO-CH2-CH2-CH2-OH
1.3%	1.4e-11	6		CH3-CH(CH3)-CH2-CO-CH3
1.2%	1.9e-11	8		CH3-CH(OH)-CH2-CH2-CO-CH2-CH2-CH3
1.1%	1.9e-11	8		CH3-CH2-CH2-CH(OH)-CH2-CH2-CO-CH3
1.1%	2.0e-11	9	PROD2-5	CH3-CH2-CH2-CH(OH)-CH2-CH2-CO-CH2-CH3
1.1%	1.9e-11	7		CH3-CH(OH)-CH(CH3)-CH2-CO-CH3
1.1%	2.2e-11	10		CH3-CH(OH)-CH2-CH2-CO-CH2-CH2-CH2-CH2-CH3
1.0%	2.2e-11	9		CH3-CH2-CH(OH)-CH2-CH2-CO-CH2-CH2-CH3
1.0%	1.4e-11	4		CH3-CO-CH2-CH2-OH
1.0%	2.2e-11	8		CH3-CH2-CH(OH)-CH(CH3)-CH2-CO-CH3
0.8%	1.9e-11	8		CH3-CH(CH3)-CH(OH)-CH2-CH2-CO-CH3
0.8%	2.0e-11	9		CH3-CH2-CH2-CH2-CH(OH)-CH2-CH2-CO-CH3
0.8%	7.4e-12	8		CH3-C(CH3)(OH)-CH2-CH(CH3)-CO-CH3
0.7%	5.5e-12	6		CH3-CO-CH2-C(CH3)(OH)-CH2-OH
0.7%	1.7e-11	8		CH3-CH(OH)-CH2-CH(CH3)-CO-CH2-CH3
0.7%	1.7e-11	7		*CH(CH3)-CH2-CH2-CH2-CO-CH2-*
0.7%	1.6e-11	7		CH3-CH(OH)-CH2-CH(CH3)-CO-CH3
0.7%	8.5e-12	9		CH3-CH2-CH2-C(CH3)(OH)-CH2-CH2-CO-CH3
22.5%				All Others

[a] Amount of formation of this compound relative to all products represented as PROD2, on a molar basis.

[b] OH radical rate constant estimated using structure-reactivity methods of Kwok and Atkinson (1995), as updated by Kwok et al (1996), in units of cm^3 $molec^{-1}$ sec^{-1}.

[c] Number of carbons.

[d] Detailed model species name used when computing mechanism for compound that was used for deriving PROD2 mechanism for the model.

[e] Product structure as used in the mechanism generation system. See Section ??. The "*" symbol is used to indicate groups that are bonded in cyclic compounds. Underlined structures are those used to derive the PROD2 mechanism.

Table 7. Product compounds predicted to be formed in the atmospheric reactions of compounds in the base ROG mixture that are represented by the RNO3 model species.

Cont'n [a]	kOH [b]	nC [c]	Model Species [d]	Product Structure [e]
	8.5e-12	6.95		Average of all Products
7.1%	1.6e-12	4		CH3-CH(ONO2)-CH2-CH3
3.3%	3.0e-12	5		CH3-CH(CH3)-CH(ONO2)-CH3
3.0%	3.0e-12	5		CH3-CH(ONO2)-CH2-CH2-CH3
2.8%	4.2e-13	3		CH3-CH(ONO2)-CH3
2.7%	1.7e-12	5		CH3-C(CH3)(ONO2)-CH2-CH3
1.8%	8.5e-12	6	RNO3-1	CH3-CH2-CH2-CH2-CH(ONO2)-CH2-OH
1.6%	2.8e-12	5		CH3-CH2-CH(ONO2)-CH2-CH3
1.1%	4.7e-12	6		CH3-CH(ONO2)-CH(CH3)-CH2-CH3
1.1%	1.2e-11	5		CH3-CH(ONO2)-CH(OH)-CH2-CH3
1.1%	1.0e-11	5		CH3-CH(OH)-CH(ONO2)-CH2-CH3
1.1%	9.9e-12	7		CH3-CH2-CH2-CH2-CH2-CH(ONO2)-CH2-OH
1.0%	4.4e-12	6		CH3-CH(CH3)-CH2-CH(ONO2)-CH3
1.0%	3.1e-12	6		CH3-C(CH3)(ONO2)-CH2-CH2-CH3
1.0%	4.2e-12	6		CH3-CH(CH3)-CH(ONO2)-CH2-CH3
1.0%	4.5e-12	4		CH3-C(CH3)(ONO2)-CH2-OH
1.0%	9.9e-12	10		CH3-CH2-CH(ONO2)-CH2-CH2-CH2-CH2-CH2-CH2-CH3
1.0%	9.9e-12	10		CH3-CH2-CH2-CH(ONO2)-CH2-CH2-CH2-CH2-CH2-CH3
1.0%	9.9e-12	10		CH3-CH2-CH2-CH2-CH(ONO2)-CH2-CH2-CH2-CH2-CH3
0.9%	5.6e-12	8	RNO3-2	CH3-CH(CH3)-CH2-C(CH3)(ONO2)-CH2-CH3
0.9%	2.8e-12	6		CH3-CH2-C(CH3)(ONO2)-CH2-CH3
0.8%	7.2e-12	6		*CH(ONO2)-CH2-CH2-CH2-CH2-CH2-*
0.8%	1.0e-11	10		CH3-CH(ONO2)-CH2-CH2-CH2-CH2-CH2-CH2-CH2-CH3
0.8%	4.2e-12	6		CH3-CH2-CH(ONO2)-CH2-CH2-CH3
0.7%	4.2e-12	7		CH3-CH2-C(CH3)(ONO2)-CH2-CH2-CH3
0.7%	6.2e-12	8		CH3-C(CH3)(ONO2)-CH2-CH(CH3)-CH2-CH3
0.7%	8.9e-12	4		CH3-CH(OH)-CH(ONO2)-CH3
0.7%	5.6e-12	7	RNO3-3	CH3-CH2-CH(ONO2)-CH2-CH2-CH2-CH3
0.7%	1.9e-11	10		CH3-CH2-CH(OH)-CH2-CH2-CH(ONO2)-CH2-CH2-CH2-CH3
0.7%	4.4e-12	6		CH3-CH(ONO2)-CH2-CH2-CH2-CH3
0.6%	3.1e-12	6		CH3-C(CH3)(ONO2)-CH(CH3)-CH3
0.6%	1.3e-11	9		CH3-CH2-CH2-CH2-CH2-CH2-CH2-CH(ONO2)-CH2-OH
0.6%	1.9e-11	10		CH3-CH2-CH2-CH(OH)-CH2-CH2-CH(ONO2)-CH2-CH2-CH3
0.6%	2.2e-12	6		CH3-C(CH3)(OH)-CH2-CH(ONO2)-CH3
0.6%	5.9e-12	7		CH3-CH(ONO2)-CH2-CH2-CH2-CH2-CH3
0.6%	3.7e-12	5		*CH(ONO2)-CH2-CH2-CH2-CH2-*
54.3%				All Others

[a] Amount of formation of this compound relative to all products represented as RNO3, on a molar basis.

[b] OH radical rate constant estimated using structure-reactivity methods of Kwok and Atkinson (1995), as updated by Kwok et al (1996), in units of cm^3 $molec^{-1}$ sec^{-1}.

[c] Number of carbons.

[d] Detailed model species name used when computing mechanism for compound that was used for deriving the RNO3 mechanism for the model.

[e] Product structure as used in the mechanism generation system. See Section ??. The "*" symbol is used to indicate groups that are bonded in cyclic compounds. Underlined structures are those used to derive the RNO3 mechanism.

In the case of PROD2, the average OH radical rate constant is 1.56 x 10^{-11} cm^3 $molec^{-1}$ s^{-1}, and the average carbon number is slightly over 7. For the purpose of deriving a PROD2 mechanism in the model, five individual compounds, indicated by being underlined on Table 6, were chosen as being representative of the entire set. The choice was largely subjective, but was made such that the average OH rate constant and the average number of carbons was approximately the same as the average, and so they included examples of different types of compounds on the list. For each of these five compounds the reaction mechanism with OH and photolysis was generated using the mechanism estimation/generation procedure discussed in Section ??, and the PROD2 parameters were derived by averaging the values obtained, weighing each of the five compounds equally[3]. Since most of these compounds are ketones, the ketone (i.e., MEK) absorption cross sections and quantum yields were used for the photolysis reactions. The mechanisms derived for these representative individual compounds are included with the mechanism listings for the detailed model species, given in Section ??. Note that although the PROD2 mechanism is derived based on a set of model species with average carbon numbers of 7, this is represented as having 6 carbons in the mechanism for the purpose of computing carbon balance.

In the case of RNO3, the average OH radical rate constant is 8.5 x 10^{-12} cm^3 $molec^{-1}$ s^{-1}, and the average carbon number is also around 7. The RNO3 mechanism in the model is derived by choosing one representative compound each for carbon numbers of 6, 7, and 8, such that the average OH rate constant is close to the average for the mixture. The compounds chosen are indicated by being underlined on Table 7. The mechanisms for these three compounds were generated and the product yield parameters obtained[3] were averaged (weighing each equally) to obtain the product yields for the reactions of RNO3. The rate of photolysis is estimated by using the absorption cross sections given by IUPAC (Atkinson et al, 1997a, 1999) for isopropyl nitrate, assuming unit quantum yield for production for NO_2.

c. Uncharacterized Aromatic Ring Fragmentation Products

Despite considerable progress in recent years towards understanding aromatic reaction mechanism (e.g., see Atkinson, 1999, and references therein), there is still insufficient information about the ring-opening products formed with OH radicals react with aromatic compounds to determine the appropriate mechanism for atmospheric modeling. In particular, the observed α-dicarbonyl and ring-retaining products from the aromatics are insufficient to account for the observed reactivity of aromatics in environmental chamber experiments, and it is necessary to assume formation of products that photolyze relatively rapidly to form radicals for model simulations to fit the environmental chamber data (e.g. Carter, 1990). To fit the data, the Carter (1990) mechanism included model species AFG1 and AFG2 to represent the contribution to reactivity of these uncharacterized ring-fragmentation products, with their yields and approximate photolysis rates adjusted to fit chamber data. Their mechanisms were based roughly on those for glyoxal and methyl glyoxal, respectively, although their action spectrum had a greater short wavelength contribution [eventually being based on that for acrolein (Carter et al, 1993b; Carter, 1995)] in order to fit reactivity data using differing types of light sources. More recently, to fit new aromatics environmental chamber data obtained using Teflon chambers with a xenon arc light source, it was found that it was also necessary to represent at least portion of the uncharacterized ring-opening products by model species with α-dicarbonyl action spectra (Carter et al, 1997a). These were represented in the model by methyl glyoxal – i.e., by increasing the methyl glyoxal yield by an adjustable amount in order to fit the chamber data (Carter et al, 1997a).

[3] The mechanisms derived for these representative individual compounds are included with the mechanism listings for the detailed model species, given in Section ??. The detailed model species names assigned to them are indicated on Tables 6 or 7.

In this version of the mechanism, the general approach of using photoreactive model species with yields adjusted to fit the chamber data to represent the effects of unknown reactive aromatic ring fragmentation products is retained. However, the number of model species used for this purpose was increased to three, and their mechanisms were derived to be somewhat more consistent with the actual types of species expected to be involved. However, the mechanisms of the model species used were changed to be more consistent with the actual types of unsaturated dicarbonyl species expected to be involved, with their names being changed from AFGn to DCBn. A third model species (DCB3) was added to allow for separate representation of products with action spectra like α-dicarbonyls, and thus end the use the methyl glyoxal model species (MGLY) for this purpose. This was done so that the mechanism used may be more appropriate for an unsaturated carbonyl, and so model predictions of MGLY will actually represent methyl glyoxal and similar species. These are discussed in more detail below[4].

DCB1 is used to represent the uncharacterized ring-opening products that do not undergo significant photodecomposition to form radicals. This includes not only the ring fragmentation formed from benzene and naphthalene, but also unsaturated diketones such as 3-hexene-2,5-dione, which the data of Bierbach et al (1994) and Tuazon et al (??) do not undergo significant radical-forming photodecomposition. This non-photoreactive model species replaces the AFG1 used in the previous versions of the mechanism to represent the uncharacterized ring-fragmentation products from benzene because fits to the benzene - NO_x chamber data are not significantly improved if it is assumed that there are other photoreactive ring-opening products besides glyoxal. This is contrast with the previous version of the mechanism, where significant photolysis of AFG1 to radicals had to be assumed to fit these data. This change is because benzene also forms glyoxal, whose photolysis to radicals was increased significantly in this version of the mechanism in order to be consistent with new chamber data on the reactivity of acetylene (Carter et al, 1997c). Also, the reaction of this species with O_3 is an additional radical source that was not in the previous mechanism.

This species is also used in the mechanisms of the alkylbenzenes because at least some of the ring-opening products are expected to have low photoreactivity, yet are expected to react rapidly by other means, particularly with OH. In particular, o-substituted aromatics such as o-xylene and 1,2,4-trimethylbenzene are expected to form higher yields of unsaturated diketones, which as indicated above do not seem to be highly photoreactive (Bierbach et al, 1994; Tuazon et al, ??). The fact that these o-substituted aromatics have relatively low reactivity in environmental chamber experiments, and that lower yields photoreactive products that give best fits to these data (Carter et al, 1997a), is consistent with the expected lower photoreactivity of these compounds. As discussed in Section ??, the yield of DCB1 is determined by assuming that the sum of all the DCBs (DCB1 + DCB2 + DCB3) is equal to the total ring fragmentation route, where the yields of the photoreactive DCB1 and DCB2 being determined by optimization. Note that this means the DCBs are used represent co-products formed with the measured α-dicarbonyls, as well as products formed in non-α-dicarbonyl-forming fragmentation routes.

The DCB1 reactions are based roughly on those estimated for HCOCH=CHCHO, with OH and O_3 rate constants based on the data of Bierbach et al (1994), and the mechanisms derived as discussed in Footnotes to Table 2. Although an OH reaction mechanism for an unsaturated diketone product such as might be formed from o-substituted aromatics may be somewhat different than that expected for 2-butene 1,4-dial, best fits to the p-xylene and 1,2,4-trimethylbenzene chamber data are obtained if the present DCB1 + OH mechanism is used.

[4] See also Section ?? for a discussion of the derivations of the yields and photolysis rates of these species based on model simulations of the aromatic - NO_x chamber experiments.

DCB2 and DCB3 are used to represent the highly photoreactive ring-opening products formed from alkylbenzenes. As discussed by Carter et al (1997a), to fit chamber data using various light sources, it is necessary to assume two separate model species for this purpose, one with an action spectrum like acrolein, and the other with an action spectrum like an α-dicarbonyl. DCB2 is used to represent those compounds with action spectra like α-dicarbonyls, and thus uses absorption cross sections of methyl glyoxal, with a wavelength-independent overall quantum yield adjusted to give best fits to the chamber data as discussed in Section ??. Likewise, DCB3 uses the absorption cross sections of acrolein, with the overall quantum yield adjusted to fit the same chamber data. Note that the overall "quantum yield" used in the model for DCB3 is greater than unity, indicating that the absorption cross sections of the actual compounds being represented must be significantly greater than those for acrolein. However, in view of lack of information concerning the nature of these compounds and their photolysis reactions, it is assumed that the wavelength dependence of the action spectra are approximately the same as that for acrolein.

Other than the photolysis rates, the reactions of DCB2 and DCB3 are the same. They are based roughly on estimated mechanisms for $CH_3C(O)CH=CHCHO$. The rate constant for the OH reaction was assumed to be the same as that used for DCB1, with the mechanism estimated as indicated in footnotes to Table 2. Because of the rapid photolysis, it is assumed that consumption of these species by reaction with O_3 is negligible. The photolysis mechanisms are unknown, and are probably highly variable depending on the individual species involved. In this mechanism, these are very approximately represented by an estimated set of products is used which gives reasonably good performance in model simulations of available chamber data (see Section ??).

d. Unreactive Product Species

The mechanism has several model species whose subsequent reactions are ignored, either because they are unreactive or because the effects of their gas-phase reactions are expected to be small. These also include "counter species" for the purpose of tracking carbon and nitrogen balance. Since their computed concentrations do not effect transformations of any of the other gas-phase species, they could be eliminated from the model if their concentrations, or tracking carbon or nitrogen balance, are not of interest.

Formic Acid (HCOOH), Acetic Acid (CCO-OH), Lumped Higher Organic Acids (RCO-OH), Peroxy Acetic Acid (CCO-OOH), and Lumped Higher Organic Peroxy Acids (RCO-OOH). Formic acid is predicted to be formed in the reactions of formaldehyde with HO_2, acetic and higher organic acids are predicted to be formed from the reactions of acyl peroxy radicals with other peroxy radicals, and peroxy acetic and higher peroxy acids are predicted to be formed when acyl peroxy radicals react with HO_2. In addition, formation of formic and higher organic acids are assumed to be the major fate of stabilized Crigiee biradicals (Atkinson, 1997a, 1999). Their subsequent reactions with OH radicals is assumed to be negligible compared to other loss processes such as deposition, though the reaction with OH may in fact be non-negligible for the higher acids or peroxy acids. Formation of these acids is included in the model because of their potential involvement in acid deposition. Depending on the model application, it may be appropriate to remove them from the model or lump them into a single organic acid species.

Carbon Dioxide (CO2). Since CO_2 does not undergo gas-phase reactions and its formation is not expected to have any other effects on the environment (since background CO_2 concentrations are much higher), the only reason for having this species in the model is carbon balance.

Unreactive Carbon (NROG). This model species is used to represent emitted VOCs or VOC oxidation products whose subsequent reactions are assumed to be negligible, and which are not otherwise represented in the model. It can be removed from the model if carbon balance is not of interest. It is represented as having one carbon, with the other carbons in the unreactive VOC or product being represented by the "lost carbon" species.

Lost Carbon (XC). The lost carbon model species is used to account for carbons that are lost (or gained) if the model species has a different number of carbons than the VOC or VOC products being represented. Note that this is different from the "unreactive carbon" (NROG) model species in that the former is used to represent *molecules* that are treated as unreactive, while the latter represents *parts of molecules* that are not being represented (i.e., that are "lost") as a result of the mechanism condensation processes. This model species can be removed in model applications where carbon balance is not of interest.

Lost Nitrogen (XN). This model species is analogous to the lost carbon (XC) species except that in this case it is used for nitrogen balance. It is not recommended that this be removed from the mechanism, so that nitrogen balance can always be verified in any model simulation. Because of the importance of nitrogen species in affecting not only O_3 formation but also radical cycles and chain lengths, any modeling system that does not maintain proper nitrogen balance must be considered to be unreliable.

Hydrogen (H2). The mechanism includes the formation of H_2 from the photolysis of formaldehyde, but the subsequent reaction of H_2 with OH is ignored because of the low rate constant and the relatively small amount formed. Tracking H_2 in the model is useful only for mechanism evaluation studies if instrumentation to measure H_2 is available, and can be eliminated from the model for ambient simulations or other applications.

Sulfates (SULF). The SULF model species is used to represent the formation of SO_3 from the reactions of SO_2 with OH. It is assumed that the fate of SO_3 in the atmosphere would be formation of sulfate aerosol. This model species would be important in models for secondary aerosol formation in scenarios where SO_2 is emitted, but could be removed if aerosols are not represented in the model application.

B. Representation Detailed Model Species

1. Listing of Detailed Model Species and Initial Reaction Rates

2. Lumped Molecule Representations

3. Generated Mechanisms

a. VOCs Represented using Generated Mechanisms

b. **Operation of Mechanism Generation System**

c. **Overview of Algorithm**

d. **Lumping Rules**

4. **Reactions of Aromatics**

5. **Reactions of Other VOCs**

a. **Isoprene, Isoprene Products, and Acroleins**

b. **Alkynes**

c. **Approximately Represented VOCs**

C. Estimation Methods

1. **Estimation of Initial Reaction Rates**

a. **OH Radical Reaction**

b. **O_3 Reaction**

c. **NO_3 Radical Reaction**

d. **O^3P Rate Constants**

e. **Photolysis Rates**

2. **Alkyl Radical and other "Fast" Reactions**

3. **Estimation of Nitrate Yields from Peroxy + NO**

4. **Estimation of Alkoxy Radical Reactions**

    a. **Reaction with O_2**

    b. **Beta Scission Decomposition**

    c. **H-Shift Isomerizations**

    d. **Other Reactions**

5. **Assigned Rate Constants and Branching Ratios**

IV. REFERENCES

Aschmann, S. M. and R. Atkinson (1998): "Kinetics of the Gas-Phase Reactions of the OH Radical with Selected Glycol Ehters, Glycols, and Alcohols," Int. J. Chem. Kinet, in press.

Atkinson, R. (1989): Kinetics and Mechanisms of the Gas-Phase Reactions of the Hydroxyl Radical with Organic Compounds," J. Phys. Chem. Ref. Data, Monograph no 1.

Atkinson, R. (1990): "Gas-Phase Tropospheric Chemistry of Organic Compounds: A Review," Atmos. Environ., 24A, 1-24.

Atkinson, R. (1994): "Gas-Phase Tropospheric Chemistry of Organic Compounds," J. Phys. Chem. Ref. Data, Monograph No. 2.

Atkinson, R. (1997a): "Gas Phase Tropospheric Chemistry of Volatile Organic Compounds: 1. Alkanes and Alkenes," J. Phys. Chem. Ref. Data, 26, 215-290.

Atkinson, R. (1997b): "Atmospheric Reactions of Alkoxy and Beta-Hydroxyalkoxy Radicals," Int. J. Chem. Kinet., 29, 99-111.

Atkinson, R. (1999): "Atmospheric Chemistry of VOCs and NO_x," Atmospheric Environment, in press. The draft article can be downloaded from the NARSTO web site at http: //www.cgenv.com/Narsto/assess_activities.html.

Atkinson, R. and S.M. Aschmann (1986): Int J. Chem. Kinet. 18, 569.

Atkinson, R. and S.M. Aschmann (1987): Atmos. Environ. 21, 2323.

Atkinson, R. and S.M. Aschmann (1988a): Int J. Chem. Kinet. 20, 513.

Atkinson, R., and S. M. Aschmann (1988b): Int. J. Chem. Kinet, 20, 1988.

Atkinson, R. and W. P. L. Carter (1984): "Kinetics and Mechanisms of the Gas-Phase Reactions of Ozone with Organic Compounds under Atmospheric Conditions," Chem. Rev. 84, 437-470.

Atkinson, R., and W. P. L. Carter (1995): "Measurement of OH Radical Reaction Rate Constants for Purasolv ELS and Purasolv ML and Calculation of Ozone Formation Potentials," Final Report to Purac America, Inc., June.

Atkinson, R. and A. C. Lloyd (1984): J. Phys. Chem. Ref. Data 13, 315.

Atkinson, R., R.A. Perry, and J. N. Pitts, Jr. (1978): J. Chem. Phys. 68, 1850.

Atkinson, R., S. M. Aschmann, W. P. L. Carter and J. N. Pitts, Jr. (1982): Int J. Chem. Kinet. 14, 839, 1982.

Atkinson, R., S. M. Aschmann and J. N. Pitts, Jr. (1983): Int. J. Chem. Kinet. 15, 75.

Atkinson, R., S. M. Aschmann, A. M. Winer and J. N. Pitts, Jr. (1985). Arch Environ. Contamin. Toxicol. 14, 417.

Atkinson, R., S. M. Aschmann, and M. A. Goodman (1987): Int. J. Chem. Kinet., 19, 299.

Atkinson, R., D. L. Baulch, R. A. Cox, R. F. Hampson, Jr., J. A. Kerr, and J. Troe (1992): "Evaluated Kinetic and Photochemical Data for Atmospheric Chemistry. Supplement IV (IUPAC)," J. Phys. Chem. Ref. Data 21, 1125-1568.

Atkinson, R., D. L. Baulch, R. A. Cox, R. F. Hampson, Jr., J. A. Kerr, M. J. Rossi, and J. Troe (1997a): "Evaluated Kinetic, Photochemical and Heterogeneous Data for Atmospheric Chemistry: Supplement V., (IUPAC)" J. Phys. Chem. Ref. Data, 26, 521-1011.

Atkinson, R., D. L. Baulch, R. A. Cox, R. F. Hampson, Jr., J. A. Kerr, M. J. Rossi, and J. Troe (1997b): "Evaluated Kinetic, Photochemical and Heterogeneous Data for Atmospheric Chemistry: Supplement VI., (IUPAC)" J. Phys. Chem. Ref. Data, 26, 1329-1499.

Atkinson, R., D. L. Baulch, R. A. Cox, R. F. Hampson, Jr., J. A. Kerr, M. J. Rossi, and J. Troe (1999): "Evaluated Kinetic, Photochemical and Heterogeneous Data for Atmospheric Chemistry: Supplement VII, Organic Species., (IUPAC)" J. Phys. Chem. Ref. Data, in press.

Batt and Robinson (1987): Int. J. Chem. Kinet. 19, 391.

Bennett, P. J. and J. A. Kerr (1989): J. Atmos. Chem. 8, 97.

Reactions of aromatic ring-opening products: Bierbach et al (1994)

Baulch, D. L., I. M. Campbell, S. M. Saunders, and P. K. K. Louie (1989): J. Chem. Soc. Faraday. Trans. 2, 85, 1819.

Bridier, I., H. Caralp, R. Loirat, B. Lesclaux and B. Veyret (1991): "Kinetic and Theoretical Studies of the Reactions of CH3C(O)O2 + NO2 + M <=> CH3C(O)O2NO2 + M between 248 and 393 K and between 30 and 760 Torr," J. Phys. Chem. 95, 3594-3600.

CALGRID DOCUMENTATION

CARB (1993): "Proposed Regulations for Low-Emission Vehicles and Clean Fuels -- Staff Report and Technical Support Document," California Air Resources Board, Sacramento, CA, August 13, 1990. See also Appendix VIII of "California Exhaust Emission Standards and Test Procedures for 1988 and Subsequent Model Passenger Cars, Light Duty Trucks and Medium Duty Vehicles," as last amended September 22, 1993. Incorporated by reference in Section 1960.

Canosa-Mass et al (1996): J. Chem. Soc. Faraday Trans. 92, 2211.

Carter, W. P. L. (1987): "An Experimental and Modeling Study of the Photochemical Reactivity of Heatset Printing Oils," Report #2 on U. S. EPA Cooperative Agreement No. CR810214-01.

Carter, W. P. L. (1988): "Development and Implementation of an Up-To-Date Photochemical Mechanism for Use in Airshed Modeling," Final Report for California Air Resources Board Contract No. A5-122-32, October.

Carter, W. P. L. (1990): "A Detailed Mechanism for the Gas-Phase Atmospheric Reactions of Organic Compounds," Atmos. Environ., 24A, 481-518.

Carter, W. P. L. (1994a): "Development of Ozone Reactivity Scales for Volatile Organic Compounds," J. Air & Waste Manage. Assoc., 44, 881-899.

Carter, W. P. L. (1994b): "Calculation of Reactivity Scales Using an Updated Carbon Bond IV Mechanism," Report Prepared for Systems Applications International Under Funding from the Auto/Oil Air Quality Improvement Research Program, April 12.

Carter, W. P. L. (1995): "Computer Modeling of Environmental Chamber Measurements of Maximum Incremental Reactivities of Volatile Organic Compounds," Atmos. Environ., 29, 2513-2517.

Carter, W. P. L. (1996): "Condensed Atmospheric Photooxidation Mechanisms for Isoprene," Atmos. Environ., 30, 4275-4290.

Carter, W. P. L (1998):. "Estimation of Atmospheric Reactivity Ranges for Parachlorobenzotrifluoride and Benzotriflouride," Report to Occidental Chemical Corporation, March.

DISCUSSION OF ESTIMATION / GENERATION SYSTEM, in preparation: Carter (1999a)

DISCUSSION OF ALKENE REACTIONS, in preparation: Carter (1999B)

Carter, W. P. L., and R. Atkinson (1985): "Atmospheric Chemistry of Alkanes", J. Atmos. Chem., 3, 377-405, 1985.

Carter, W. P. L. and R. Atkinson (1996): "Development and Evaluation of a Detailed Mechanism for the Atmospheric Reactions of Isoprene and NOx," Int. J. Chem. Kinet., 28, 497-530.

Carter, W. P. L., and F. W. Lurmann (1990): "Evaluation of the RADM Gas-Phase Chemical Mechanism," Final Report, EPA-600/3-90-001.

Carter, W. P. L. and F. W. Lurmann (1991): "Evaluation of a Detailed Gas-Phase Atmospheric Reaction Mechanism using Environmental Chamber Data," Atm. Environ. 25A, 2771-2806.

Carter, W. P. L., F. W. Lurmann, R. Atkinson, and A. C. Lloyd (1986): "Development and Testing of a Surrogate Species Chemical Reaction Mechanism," EPA-600/3-86-031, August.

Carter, W. P. L., R. Atkinson, A. M. Winer, and J. N. Pitts, Jr. (1982): "Experimental Investigation of Chamber-Dependent Radical Sources," Int. J. Chem. Kinet., 14, 1071.

Carter, W. P. L., Winer, A. M., Atkinson, R., Dodd, M. C. and Aschmann, S. A. (1984): Atmospheric Photochemical Modeling of Turbine Engine Fuels. Phase I. Experimental studies. Final Report to the USAF, ESL-TR-84-32, September.

Carter, W. P. L., A. M. Winer, R. Atkinson, S. E. Heffron, M. P. Poe, and M. A. Goodman (1987): "Atmospheric Photochemical Modeling of Turbine Engine Fuels. Phase II. Computer Model Development," Report on USAF Contract no. F08635-83-0278.

Carter, W. P. L., J. A. Pierce, I. L. Malkina, and D. Luo (1992): "Investigation of the Ozone Formation Potential of Selected Volatile Silicone Compounds," Final Report to Dow Corning Corporation, Midland, MI, November.

Carter, W. P. L., J. A. Pierce, I. L. Malkina, D. Luo and W. D. Long (1993a): "Environmental Chamber Studies of Maximum Incremental Reactivities of Volatile Organic Compounds," Report to Coordinating Research Council, Project No. ME-9, CARB, etc. [a]

Carter, W. P. L, D. Luo, I. L. Malkina, and J. A. Pierce (1993b): "An Experimental and Modeling Study of the Photochemical Ozone Reactivity of Acetone," Final Report to Chemical Manufacturers Association Contract No. KET-ACE-CRC-2.0. December 10. [a]

Carter, W. P. L., D. Luo, I. L. Malkina, and J. A. Pierce (1994): "Environmental Chamber Studies of Atmospheric Ozone Formation from Selected Biogenic Compounds" Presented at the 207th ACS National Meeting, March 13-17, San Diego, CA. [a]

Carter, W. P. L., J. A. Pierce, D. Luo, and I. L. Malkina (1995a): "Environmental Chamber Studies of Maximum Incremental Reactivities of Volatile Organic Compounds," Atmos. Environ. 29, 2499-2511.

Carter, W. P. L., D. Luo, I. L. Malkina, and J. A. Pierce (1995b): "Environmental Chamber Studies of Atmospheric Reactivities of Volatile Organic Compounds. Effects of Varying ROG Surrogate and NOx," Report to Coordinating Research Council, CARB, etc [a]

Carter, W. P. L., D. Luo, I. L. Malkina, and J. A. Pierce (1995c): "Environmental Chamber Studies of Atmospheric Reactivities of Volatile Organic Compounds. Effects of Varying Chamber and Light Source," Final report to NREL, CRC, CARB, etc. [a]

Carter, W. P. L., D. Luo, I. L. Malkina, and D. Fitz (1995d): "The University of California, Riverside Environmental Chamber Data Base for Evaluating Oxidant Mechanism. Indoor Chamber Experiments through 1993," Report submitted to the U. S. EPA [a]

Carter, W. P. L., D. Luo, and I. L. Malkina (1996a): "Investigation of Atmospheric Ozone Formation Potentials of C12 - C16 n-Alkanes," Report to the Aluminum Association, October 28. [a]

Carter, W. P. L., D. Luo, and I. L. Malkina (1996b): "Investigation of the Atmospheric Ozone Impact of Methyl Acetate," Report to Eastman Chemical Company, July. [a]

Carter, W. P. L., D. Luo, and I. L. Malkina (1996c): "Investigation of the Atmospheric Ozone Formation Potential of t-Butyl Alcohol, N-Methyl Pyrrolidinone and Propylene Carbonate," Report to ARCO Chemical Corporation, July 8. [a]

Carter, W. P. L., D. Luo, and I. L. Malkina (1996d): "Investigation of the Atmospheric Ozone Formation Potential of Trichloroethylene," Report to the Halogenated Solvents Industry Alliance, August. [a]

Carter, W. P. L., D. Luo, and I. L. Malkina (1997a): "Environmental Chamber Studies for Development of an Updated Photochemical Mechanism for VOC Reactivity Assessment," Draft final report to CARB, CRC, NREL [a]

Carter, W. P. L., D. Luo, and I. L. Malkina (1997b): "Investigation of the Atmospheric Ozone Formation Potential of Propylene Glycol," Report to Philip Morris, USA, May 2. [a]

Carter, W. P. L., D. Luo, and I. L. Malkina (1997c): "Investigation of the Atmospheric Ozone Formation Potential of Acetylene," Report to Carbind Graphite Corp., April 1. [a]

Carter, W. P. L., D. Luo, and I. L. Malkina (1997d): "Investigation of the Atmospheric Ozone Formation Potential of Selected Alkyl Bromides," Report to Albemarle Corporation, November 10. [a]

Carter, W. P. L., D. Luo, I. L. Malkina, S. M. Aschmann and R. Atkinson (1997e): "Investigation of the Atmospheric Ozone Formation Potentials of Selected Dibasic Esters," Report to the Dibasic Esters Group, SOCMA, August 29. [a]

Carter, W. P. L., D. Luo, and I. L. Malkina (1997f): "Investigation of the Atmospheric Ozone Formation Potentials of Selected Mineral Spirits Mixtures," Report to Safety-Kleen Corporation, July 25. [a]

Carter, W. P. L., D. Luo, and I. L. Malkina (1997g): "Investigation of the Atmospheric Ozone Formation Potential of t-Butyl Acetate," Report to ARCO Chemical Corporation, July 2. [a]

Carter, W. P. L., D. Luo and I. L. Malkina (1997h): "Investigation of that Atmospheric Reactions of Chloropicrin," Atmos. Environ. 31, 1425-1439.; Report to the Chloropicrin Manufacturers Task Group, May 19. [a]

Carter, W. P. L., D. Luo, and I. L. Malkina (1997i): "Investigation of the Atmospheric Ozone Formation Potential of Toluene Diisocyanate," Report to Society of the Plastics Industry, december. [a]

Carter. W. P. L. et al. (1999a): "Investigation of Atmospheric Reactivities of Selected Consumer Product VOCs," Report in preparation.

Carter, W. P. L., et al. (1999b), "An Experimental and Modeling Study of the Photochemical Reactivity of Selected C12+ Cycloalkanes," Report to the Aluminum Association, in preparation.

Carter, W. P. L., D. Luo, and I. L. Malkina (1999c): "Investigation of the Atmospheric Impacts and Ozone Formation Potential of Styrene," Report to the Styrene Information and Research Center. March 10.

Croes, B., California Air Resources Board Research Division, personal communication.

P. Dagaut, T. J. Wallington, R. Liu and M. J. Kurylo (1988a): 22nd International Symposium on Combustion, Seattle, August 14-19.

Dagaut, P., T. J. Wallington, R. Liu and J. J. Kurylo (1988b): J. Phys. Chem. 92, 4375.

OH + NO2 kinetics: Donahue et al (1997)

OH + NO2 kinetics: Forster et al (1995)

Gardner, E. P., P. D. Sperry, and J. G. Calvert (1987): J. Phys. Chem. 91, 1922.

Hartmann et al (1876). kOH (ethoxyethanol). See Carter et al (1993a).

Jeffries, H. E., K. G. Sexton, J. R. Arnold, and T. L. Kale (1989): "Validation Testing of New Mechanisms with Outdoor Chamber Data. Volume 2: Analysis of VOC Data for the CB4 and CAL Photochemical Mechanisms," Final Report, EPA-600/3-89-010b.

Jenkin, M. E., R. A. Cox, M. Emrich and G. K. Moortgat (1993): "Mechanisms for the Cl-atom-initiated Oxidation of Acetone and Hydroxyacetone in Air," J. Chem. Soc. Faraday Trans. 89, 2983-2991.

HO2 + HO2 data: Kircher and Sander (1984)

Kirchner, F. and W. R. Stockwell (1996): "Effect of Peroxy Radical Reactions on the Predicted Concentrations of Ozone, Nitrogenous Compounds, and Radicals," J. Geophys. Res. 101, 21,007-21,022.

Kirchner, F., F. Zabel and K. H. Becker (1992): "Kinetic Behavior of Benzoylperoxy Radicals in the Presence of NO and NO2," Chem. Phys. Lett. 191, 169-174.

Kwok, E. S. C., and R. Atkinson (1995): "Estimation of Hydroxyl Radical Reaction Rate Constants for Gas-Phase Organic Compounds Using a Structure-Reactivity Relationship: An Update," Atmos. Environ 29, 1685-1695.

Kumar, N., F. W. Lurmann, and W. P. L. Carter (1995), "Development of the Flexible Chemical Mechanism Version of the Urban Airshed Model," Report to California Air Resources Board, Agreement no. 93-716. Document No. STI-94470-1508-FR, Sonoma Technology, Inc. Santa Rosa, CA, August.

Estimation method updates: Kwok et al (1996)

Langford, A. O, and C. B. Moore (1984): J. Chem. Phys. 80, 4211.

NO3 + HV data. Magnotta and Johnsom (1980)

NO3 + HO2 reaction: Mellouki et al (1993)

NASA (1994): "Chemical Kinetics and Photochemical Data for Use in Stratospheric Modeling, Evaluation Number 11," JPL Publication 94-26, Jet Propulsion Laboratory, Pasadena, California, December.

NASA (1997): "Chemical Kinetics and Photochemical Data for Use in Stratospheric Modeling, Evaluation Number 12," JPL Publication 97-4, Jet Propulsion Laboratory, Pasadena, California, January.

H. Niki, P. D. Maker, C. M. Savage, and L. P. Breitenback (1985): Int. J. Chem. Kinet. 17, 347.

Majer, Naman, and Robb (1969): Trans. Faraday Soc, 65 1846.

Mentel et al (1996) N2O5 + H2O Chamber Study

PPN Kinetics: Mineshos and Glavas (1991)

Paulson, S. E., J. J. Orlando, G. S. Tyndall, and J. G. Calvert (1995): Int. J. Chem. Kinet. 27, 997.

Pitts, J. N., Jr., K. Darnall, W. P. L. Carter, A. M. Winer, and R. Atkinson (1979): "Mechanisms of Photochemical Reactions in Urban Air," EPA-600/ 3-79-110, November.

Plum, C. N., Sanhuesa, E., Atkinson, R., Carter W. P. L. and Pitts, J. N., Jr. (1983): "OH Radical Rate Constants and Photolysis Rates of alpha-Dicarbonyls," Environ. Sci. Technol. 17, 479-484.

Porter, E., G. Locke, J. Platz, J. Treacy, H. Sidebottom, W. Mellouki, S. Teton, and G. LeBras. (1995): "Kinetics and Mechanisms for the OH Radical Initiated Oxidation of Oxygenated Organic Compounds," Workshop on Chemical Mechanisms Describing Oxidation Processes in the Troposphere, Valencia, Spain, April 25-28.

Saunders et al (1994). K(OH + t-butanol)

Roberts, J. M. and S. B. Bertman (1992): Int J. Chem. Kinet. 24, 297.

PPN Kinetics: Schurath and Wipprecth (1980)

Sidebottom, H. W., G. LeBras, K. H. Becker, J. Wegner, E. Porter, S. O'Donnell, J. Morarity, E. Collins, A. Mellouki, S. Le Calve, I. Barnes, C. Sauer, K. Wirtz, M. Martin-Revejo, L. Theuner and J. Bea (1997): "Kinetics and Mechanisms for the Reaction of Hydroxyl Radicals with $CH_3OCH_2OCH_3$ and Related Compounds," Final Report to Lambiotte & Cie, S.A., September.

Vinyl + O2 reaction: Slagle et al (1984)

Smith, D. F, T. E. Kleindienst, E. E. Hudgens, C. D. McIver and J. J. Bufalini (1992): Int. J. Chem. Kinet. 24, 199.

Stemmler, K. D. J. Kinnison and J. A. Kerr (1996): J. Phys. Chem, 100, 2114.

Stockwell, W. R., P. Middleton, J. S. Chang, and X. Tang (1990): "The Second Generation Regional Acid Deposition Model Chemical Mechanism for Regional Air Quality Modeling," J. Geophys. Res. 95, 16343- 16376.

Stockwell, W.R., F. Kirchner, M. Kuhn, and S. Seefeld (1997): A new mechanism for regional atmospheric chemistry modeling. J. Geophys. Res., 102, 25847-25880.

HONO Quantum Yields (Stockwell and Calvert, 1978)

Tuazon, E. C., W. P. L. Carter and R. Atkinson (1991): "Thermal Decomposition of Peroxyacetyl Nitrate and Reactions of Acetyl Peroxy Radicals with NO and NO_2 Over the Temperature Range 283-313 K," J. Phys. Chem., in 95, 2434.

Tuazon, E. C., S. M. Aschmann and R. Atkinson (1998a): "Products of the Gas-Phase Reactions of the OH radical with 1-Methoxy-2-Propanol and 2-Butoxyethanol," Environ. Sci. Technol., Submitted.

Tuazon, E. C., S. M. Aschmann, R. Atkinson, and W. P. L. Carter (1998b): "The reactions of Selected Acetates with the OH radical in the Presence of NO: Novel Rearrangement of Alkoxy Radicals of Structure RC(O)OCH(O.)R'", J. Phys. Chem A 102, 2316-2321.

Tuazon et al 3-hexene-2,4-dione

Wallington, T. J. and M. J. Kurylo (1987): J. Phys. Chem 91, 5050.

Wallington, T. J., P. Dagaut, R. Liu and M. J. Kurylo (1988a): Int. J. Chem. Kinet. 20, 541.

Wallington, T. J., R. Liu, P. Dagaut, and M. J. Kurylo (1988b): Int. J. Chem. Kinet. 20, 41.

Wallington, T. J., P. Dagaut and M. J. Kurylo (1988c): J. Phys. Chem. 92, 5024.

Wallington, T. J., P. Dagaut, R. Liu, and M. J. Kurylo (1988d): Int. J. Chem. Kinet. 20, 177.

Wallington, T., J., W. O. Siegl, R. Liu, Z. Zhang, R. E. Huie, and M. J. Kurylo (1990): "The Atmospheric Reactivity of à-Methyltetrahydrofuran," Env. Sci. Technol. 24, 1568-1599.

Wells, R, et al. (1999): Submitted for publication in Int. J. Chem. Kinetics.

Reference for expanded Carbon Bond IV